STN - ainearvot

Esimerkkihaku: Metyylimerkaptaanin höyrynpaine

6.8.2013
Riitta Housh

Sisällysluettelo

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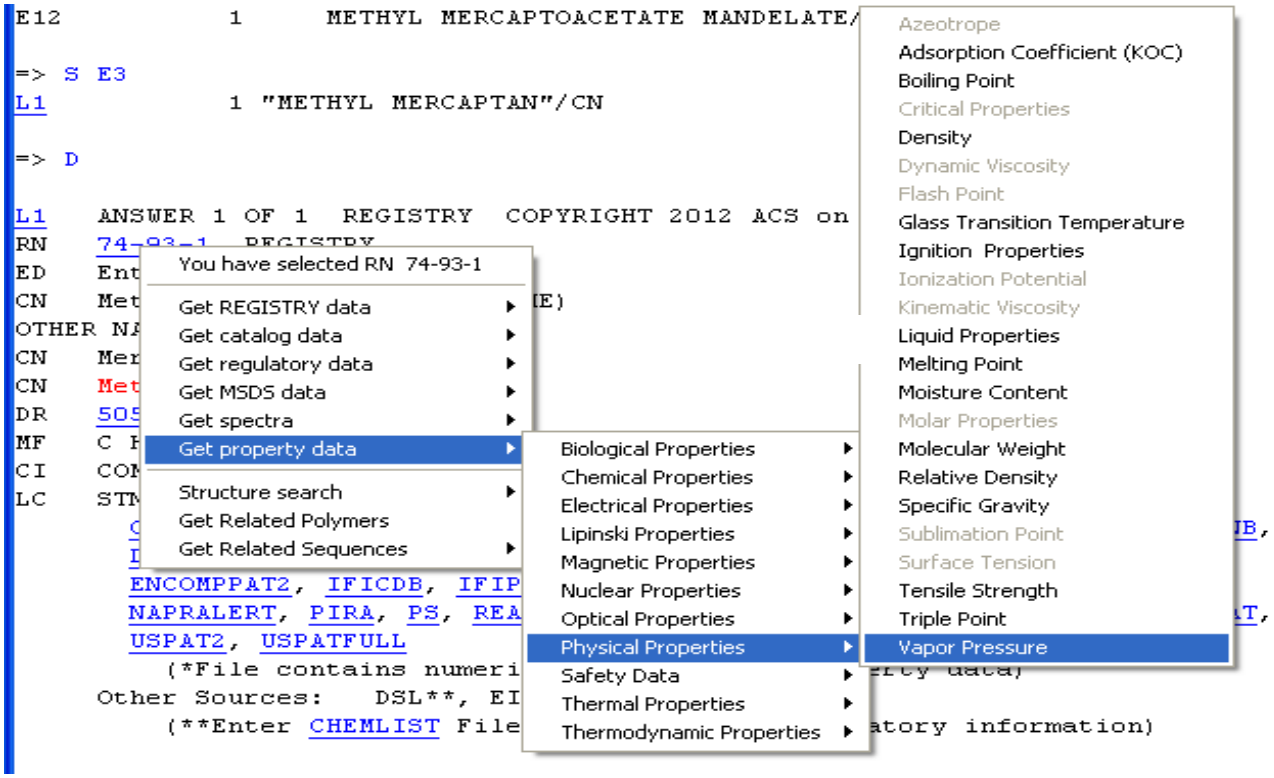
1. STN-numeeriset tietokannat

Tietokanta	Aineita	Tietueita	Vuo-desta	Yhdisteet	Sisältö - ominaisuudet
REGISTRY	65 milj (130 milj.)	65 milj. (130 milj.)	1907	Kaikki	2 miljardia kokeellista ja laskennalllista ominaisuusarvoa
REAXYSFILE	20 milj.	20 milj.	1771	Org. ja epäorg. aineet	Fysikaalisia, termodynaamisia ja EcoPharm-ominaisuuksia, spektrejä, reaktioita, patentteja ym.
CHEMSAFE	1 500	47 000		Palavat kaasut, nesteet, seokset	40 turvallisuusteknistä ominaisuutta
DETHERM	20 000 + seoksia	750 000 taulukkoa, 47000 lähdettä	1819	Epäorg. ja org. aineet, paljon seoksia	500 termofysikaalista ominaisuutta
ICSD		135 000	1913	Epäorg. yhdisteet	Rakenneparametrit
RTECS	176 000	176 000	1971	Org. ja epäorg. aineet	Toksisuus

2. Ominaisuustiedot STN Expressin automaattitoimintoa käyttäen

Huom!
REAXYSFILE on erikseen valittava mukaan asetuksista: Preferences/ STN Online and Results/Account. Ruksaa ReaxysFile kohdassa Property Databases.
DETHERM ei ole mukana, joten se pitää aina hakea erikseen komentokielellä. Kaikki ominaisuudet eivät myöskään ole mukana.

- **Kun klikkaat rekisterinumeroa hiiren vasemmalla painikkeella minkä tahansa STN:n tietokannan tietueessa, saat ruudulle seuraavia valikoita.**



- **Klikkaa Vapor Pressure**
- **Kaikki tapahtuu sen jälkeen automaattisesti.**
- **Vastaa vain kysymyksiin.**

```
=>  display set notice

SET PARAMETER CURRENT  PERMANENT LOGIN DEFAULT
------------- -------  --------- ----- -------
NOTICE (EUR)
  DISPLAY     '50'     '50'      '50'  '100'
  SEARCH      '30'     '30'      '30'  '1000'

=> FIL REGISTRY
FILE 'REGISTRY' ENTERED AT 12:08:51 ON 19 SEP 2012
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.
```

```
STRUCTURE FILE UPDATES:   18 SEP 2012  HIGHEST RN 1394891-73-6
DICTIONARY FILE UPDATES:  18 SEP 2012  HIGHEST RN 1394891-73-6

CAS Information Use Policies apply and are available at:
http://www.cas.org/legal/infopolicy


=> S 74-93-1/RN

L2           1 74-93-1/RN

=> SET SMA OFF

SET COMMAND COMPLETED

=> DEL SEL Y


=> SEL RN

E1 THROUGH E1 ASSIGNED

=> SET SMA LOGIN

SET COMMAND COMPLETED

=> INDEX REGISTRY,REAXYSFILE
INDEX 'REGISTRY, REAXYSFILE' ENTERED AT 12:08:56 ON 19 SEP 2012

2 FILES IN THE FILE LIST IN STNINDEX

Enter SET DETAIL ON to see search term postings or to view
search error messages that display as 0* with SET DETAIL OFF.

=> S E1 AND VP/FA

          1   FILE REGISTRY
          1   FILE REAXYSFILE

   2 FILES HAVE ONE OR MORE ANSWERS,    2 FILES SEARCHED IN STNINDEX

L3   QUE 74-93-1/BI AND VP/FA

=> D RANK

F1           1   REGISTRY
F2           1   REAXYSFILE


=> FIL HITS

FILE 'REGISTRY' ENTERED AT 12:09:01 ON 19 SEP 2012
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FILE 'REAXYSFILE' ENTERED AT 12:09:01 ON 19 SEP 2012
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=> S L3

L4           2 L3

=> SET NOTICE 1 DISPLAY
```

```
NOTICE SET TO 1 EURO FOR DISPLAY COMMAND
SET COMMAND COMPLETED

=> D RN CN VP 1-

YOU HAVE REQUESTED DATA FROM 2 ANSWERS - CONTINUE? Y/(N):Y
THE ESTIMATED COST FOR THIS REQUEST IS 14,57 EUROS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:Y

L4   ANSWER 1 OF 2  REGISTRY  COPYRIGHT 2012 ACS on STN
RN   74-93-1  REGISTRY
CN   Methanethiol  (CA INDEX NAME)
OTHER NAMES:
CN   Mercaptomethane
CN   Methyl mercaptan

CODE|  VALUE  |CONDITION|   TYPE    |NOTE
====+=========+=========+===========+====
VP  |2.533 bar|298 K    |Predicted |(1)

(1)  Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02
     ((C) 1994-2012 ACD/Labs)


See HELP PROPERTIES for information about property data sources in REGISTRY.


L4   ANSWER 2 OF 2 REAXYSFILE COPYRIGHT 2012 Elsevier Properties SA. on STN

     CAS Reg. No. (RN):              74-93-1
     Chemical Name (CN):             methanethiol, methyl mercaptane, methyl
                                     mercaptan, methylmercaptane,
                                     MERCAPTOMETHYLE, methylmercaptan,
                                     methylenethiol
     Autonom Name (AUN):             Methanethiol


Vapour Pressure:
 Value        | Temp.            |Ref.| Note
 (VP)         | (.T)             |    |
 (bar)        | (K)              |    |
==============+==================+====+=======
 1.5800257    | 293.15           |1   |
              |                  |2, 3|
 0.8452655 -  | 274.55 - 307.05  |4   | 1
 2.7011837    |                  |    |
 0.0349397 -  | 215.25 - 293.15  |5   | 2
 1.7003755    |                  |    |
 0.5188892 -  | 263.15 - 288.15  |6   |
 1.4292118    |                  |    |
 0.0548353 -  | 495.05 - 552.25  |7   |
 1.0141005    |                  |    |
 0.7932659    | 273.15 - 469.95  |8   |

Reference(s):
1. Lestremau, Francois; Andersson, Fraes Annika T.; Desauziers, Valerie; Fanlo,
   Jean-Louis, Analytical Chemistry, CODEN: ANCHAM, 75(11), <2003>, 2626 - 2632
2. Wolff et al., Journal of Chemical Thermodynamics, CODEN: JCTDAF, 12, <1980>,
   641,644, 645, 647, 650
3. Osborn; Scott, Journal of Chemical Thermodynamics, CODEN: JCTDAF, 12,
   <1980>, 429,434, 436
4. Osborn, A. G.; Scott, D. W., Journal of Chemical Thermodynamics, CODEN:
   JCTDAF, 12(5), <1980>, 429 - 438
5. Wolff, Hans; Szydlowski, Jerzy; Dill-Staffenberger, Ludmilla, Journal of
```

Chemical Thermodynamics, CODEN: JCTDAF, 12(7), <1980>, 641 - 652
6. Jackowski, Andrzej W., Polish Journal of Chemistry, CODEN: PJCHDQ, 54(9), <1980>, 1765 - 1773
7. Russell; Osborne; Yost, Journal of the American Chemical Society, CODEN: JACSAT, 64, <1942>, 165
8. Berthoud; Brum, Journal de Chimie Physique et de Physico-Chimie Biologique, CODEN: JCPBAN, 21, <1924>, 144

Notes(s):
1. Table exists. Equation: Y
2. Table exists. Equation: lgp=-49087.2(K/T)E2-973.974(K/T)+6.12449

=> *SET NOTICE 50 DISPLAY*

NOTICE SET TO 50 EUROS FOR DISPLAY COMMAND
SET COMMAND COMPLETED

=> **D HIS NOF**

```
     (FILE 'HOME' ENTERED AT 12:02:45 ON 19 SEP 2012)

     FILE 'REGISTRY' ENTERED AT 12:03:12 ON 19 SEP 2012
                E METHYL MERCAPTAN/CN
L1            1 SEA SPE=ON  ABB=ON  PLU=ON  "METHYL MERCAPTAN"/CN
                D
                DISPLAY SET NOTICE

     FILE 'REGISTRY' ENTERED AT 12:08:51 ON 19 SEP 2012
L2            1 SEA SPE=ON  ABB=ON  PLU=ON  74-93-1/RN
                SET SMA OFF
                DEL SEL Y
                SEL RN
                SET SMA LOGIN

     INDEX 'REGISTRY, REAXYSFILE' ENTERED AT 12:08:56 ON 19 SEP 2012
                SEA E1 AND VP/FA
               ---------
               1   FILE REGISTRY
               1   FILE REAXYSFILE
L3              QUE SPE=ON  ABB=ON  PLU=ON  74-93-1/BI AND VP/FA
               ---------
                D RANK

     FILE 'REGISTRY, REAXYSFILE' ENTERED AT 12:09:01 ON 19 SEP 2012
L4            2 SEA SPE=ON  ABB=ON  PLU=ON  L3
                SET NOTICE 1 DISPLAY
                D RN CN VP 1-
                SET NOTICE 50 DISPLAY
```

3. Ominaisuustiedot komentokieltä käyttäen

Edut automatiikkaan verrattuna

- **Saadaan mukaan myös DETHERM- ja CHEMSAFE-tietokannat**
- **Saadaan ominaisuuksia, joita automatiikka ei anna.**

Yleistä pääosalle numeerisia tietokantoja (Poikkeus DETHERM ja CHEMSAFE)

Haku

- **Kullakin yhdisteellä on yleensä vain yksi tietue, jossa annetaan kaikki saatavilla olevat ominaisuudet.**
- **Hae tietue yhdiste CAS-numeron avulla. Suositeltavinta on käyttää REGISTRYn L-numeroa, koska sliloin haku tehdään myös aineen "vanhoilla" rekisterinumeroilla.**

Tulostus

- **Älä koskaan tulosta numeerisissa tietokannoissa D ALL, ellet todella tarvitse kaikkia tietoja ja tiedä, mitä teet. Tulostus ALL -formaatilla voi tulla hyvin kalliiksi. Tarkista ensin tulostusmaksut (HELP COST).**
- **Kun tiedät, mitä haluat**
  - **Hae etsittävä ominaisuus FA (Field Availability) –kentästä. (EXPAND VAPOR/FA)**
  - **Yhdistä ominaisuus AND-operaattorilla aineen tietueeseen.**
  - **Tulosta sen jälkeen oletustulostusmuodolla (pelkkä D) (= Query Related Display), jolloin saat vain ne tiedot, joilla tietue haettiin. Voit tietysti myös tulostaa kenttätunnusten avulla. Registryssä ominaisuus pitää tulostaa kenttätunnuksen avulla, koska D antaa aina vain indentifiointitiedot.**
- **Kun et tarkkaan tiedä etsittyjen ominaisuuksien kenttäkoodeja tai mitä ominaisuuksia haluat.**
  - **Tulosta FA (Field Availaibility)-kenttä. FA ilmoittaa, mitä kenttiä (ominaisuuksia) aineelle on annettu kyseisessä tietokannassa. Se on maksuton muualla paitsi ReaxysFileissa .**
  - **Katso läpi yhdisteelle annetut ominaisuudet ja valitse listasta kiinnostavat**
  - **Tulosta haluamasi ominaisuudet suoraan kenttäkoodilla.**
  - **Myös aineen identifiointitiedot (IDE) kannattaa tulostaa samalla, jotta voi olla varma, että ominaisuudet ovat etsitylle aineelle.**

3.1 Registry

- **Hae Registry muuten kuten edellä yleisohjeessa , mutta tulosta ominaisuus kenttätunnuksella. Pelkkä D antaa vain identifiointitiedot.**

```
=> FIL REG
FILE 'REGISTRY' ENTERED AT 12:18:02 ON 19 SEP 2012
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REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:
http://www.cas.org/training/stn/database-specific

=> E METHYL MERCAPTAN/CN
E1            1     METHYL MELITRATE A/CN
E2            1     METHYL MELLOPHANATE/CN
E3            1 --> METHYL MERCAPTAN/CN
E4            1     METHYL MERCAPTAN LITHIUM SALT/CN

=> S E3
L1            1 "METHYL MERCAPTAN"/CN

=> D

L1   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2012 ACS on STN
RN   74-93-1  REGISTRY
ED   Entered STN:  16 Nov 1984
CN   Methanethiol  (CA INDEX NAME)
OTHER NAMES:
CN   Mercaptomethane
CN   Methyl mercaptan
DR   505027-72-5, 63933-47-1
MF   C H4 S
CI   COM
LC   STN Files:   AGRICOLA, ANABSTR, BIOSIS, BIOTECHNO, CA, CABA, CAPLUS,
       CASREACT, CBNB, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSNB,
       DDFU, DETHERM*, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT,
       ENCOMPPAT2, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS,
       NAPRALERT, PIRA, PS, REAXYSFILE*, RTECS*, SPECINFO, TOXCENTER, ULIDAT,
       USPAT2, USPATFULL
         (*File contains numerically searchable property data)
     Other Sources:   DSL**, EINECS**, TSCA**
         (**Enter CHEMLIST File for up-to-date regulatory information)


  H3C—SH

**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
            9201 REFERENCES IN FILE CA (1907 TO DATE)
             124 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
            9242 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> D FA

L1   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2012 ACS on STN
Available Properties (PRFA)

CODE    | PROPERTY
========+=====================
```

```
Experimental Data

BP         Boiling Point
DEN        Density
MP         Melting Point
SPEC       Carbon-13 NMR Spectra
SPEC       IR Absorption Spectra
SPEC       Mass Spectra
SPEC       Proton NMR Spectra
ETAG       Experimental Tags

Predicted Data

BCF        Bioconcentration Factor
BP         Boiling Point
DEN        Density
FP         Flash Point
FRB        Freely Rotatable Bonds
HAC        H acceptors
HD         H donors
HDAS       Hydrogen Donors/Acceptors Sum
HVAP       Enthalpy of Vaporization
ISLB.MASS  Mass Intrinsic Solubility
ISLB.MOL   Molar Intrinsic Solubility
KOC        Koc
LOGD       logD
LOGP       logP
MVOL       Molar Volume
MW         Molecular Weight
PKA        pKa
PSA        Polar Surface Area
SLB.MASS   Mass Solubility
SLB.MOL    Molar Solubility
VP         Vapor Pressure
```

Tulosta kenttätunnuksen avulla, koska D antaa aina vain identifiointitiedot

```
=> D VP

L1   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2012 ACS on STN
CODE|  VALUE  |CONDITION|   TYPE   |NOTE
====+=========+=========+==========+====
VP  |2.533 bar|298 K    |Predicted |(1)

(1)  Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02
     ((C) 1994-2012 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

=> HELP COST

 STN International Fees and Prices Effective June 9, 2012
 REGISTRY File
 -------------                                Euro
                                             ------
 Connect Hour Fee (per hour)                  35,00
 Dictionary or Property Searching (per term):
  Text or Numeric term (4)                     4,75

 Format Display and Print Fees (per answer)
  SCAN, RE, RETABLE, RECNT, PRFA              FREE
  REG                                          0,23
  IDE or FIDE or NA or SQN or
   ED (6,8)                                    1,79
  EPROP (experimental properties)              1,18
  SPEC (spectra)                               1,18
  ETAG (experimental property tags            FREE
  PPROP (predicted property data)              1,18
```

3.2 ReaxysFile

- **Samalla yhdisteellä voi olla useita tietueita ReaxysFileissa. Päätietue on yleensä viimeisin, mutta ei välttämättä**
- **Hae yhdisteen tietueet ReaxysFileissa Registry-tietokannan joukkonumeron avulla.**
- **Kaikilla yhdisteillä ei REAXYSFILEissa ole CAS-rekisterinumeroa.**
  - **Jos CAS-numerolla tai Registryn L-numerolla ei löydy mitään:**
  - **Yritä vielä yhdisteen nimellä CN (Chemical Name) -kentästä.**
  - **Kokeile myös saksankielisiä nimiä.**
  - **Voit myös hakea nimen osilla CNS (Chemical Name Segment) -kentästä.**
- **ReaxysFileiln hinnoittelu poikkeaa muista. Kaikista ominaisuustulosteista veloitetaan sama yksikkömaksu 6 euroa (v. 2013). D antaa sekä identifiointitiedot että listan saatavilla olevista tiedoita (FA = Field Availability).**
- **Jos ReaxysFileissa on useita tietueita etsimällesi yhdisteelle ja koska myös FA maksaa, niin älä tulosta kaikille D FA, vaan tee haku, jossa yhdistät yhdisteen ja ominaisuuden. Hae ominaisuus joko tietokantojen kuvailusivuilta tai STN:stä EXPAND-komennolla. (S L2 AND VP/FA)**
- **Muutamia tuloskenttiä on yhdistetty superkentiksi, joiden tulostus maksaa vain yhden yksikön. Superkenttäluettelon saa HELP COST:illa. Superkenttäkoodin avulla voit tulostaa ovat mm. kaikki termodynaamiset (THE) tai optiset (OPT) ominaisuudet yhdellä veloitusmaksulla. Käytä superkentän koodia, sillä jos luettelet alakentät erikseen, menee jokaisesta oma maksunsa.**

```
=> FIL REAXYS
FILE 'REAXYSFILE' ENTERED AT 12:18:54 ON 19 SEP 2012
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FILE RELOADED ON AUGUST 1, 2012
FILE COVERS 1771 TO 2011.

*** FILE CONTAINS 19,404,345 SUBSTANCES ***

>>> For details on preparations and reactions searching
    see  HELP PRE and HELP RXS <<<

  PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST.
  SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE
  ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE THESE
  ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.
  FOR PRICE INFORMATION SEE HELP COST

*************************************************************
* For reviewing changes and content of ReaxysFile please enter *
* HELP CHANGE, respectively HELP CONTENT at an arrow prompt.   *
*************************************************************

>>> FOR THE LATEST REAXYSFILE STN USER DOCUMENTATION,
    PLEASE VISIT:
    http://www.stn-international.com/stn_chemistry_reaxysfile.html <<<


=> S L1
L2            3 L1

=> E VAPOR/FA
```

```
E1     1215706     UV AND VISIBLE SPECTRUM/FA
E2     1215706     UVS/FA
E3           0 --> VAPOR/FA
E4        9477     VAPOUR PRESSURE/FA
E5        9477     VP/FA
E6      153863     XREF/FA
E7         638     XS/FA
**** END OF FIELD ****

=> S L2 AND E4
          9477 "VAPOUR PRESSURE"/FA
L3           1 L2 AND "VAPOUR PRESSURE"/FA

=> HELP COST

    STN International Fees and Prices, Effective Jul 28, 2012

    REAXYSFILE File                      Euro
    --------------                      -------

    Connect Hour Fee (per Hour) .      55,00
    Display Fee / Print Fee . . .       5,80
    (per billable field)

    The following superfields are billed as one fee unit.
    IDE, CRY, ECB, ECO, ELEP, GAS, LIQ, MAGP, MECP, OPTP, SEP,
    SF, SOL, THE, TRA, CHE, LVS.
    For a description and which "narrower" terms they include,
    see Summary Sheet

    Select Fee per record
    - RN . . . . . .       0,34

    This file does not participate in the STN Keep & Share Program.
    See HELP USAGETERMS for re-use permissions or contact the
    database producer.


=> D
THE ESTIMATED COST FOR THIS REQUEST IS 220,40 EUROS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:Y


L3   ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2012 Elsevier Properties SA. on STN

     Accession Number (AN):          1696840
     Basic Pref. RN (BPR):           74-93-1
     CAS Reg. No. (RN):              74-93-1
     Chemical Name (CN):             methanethiol, methyl mercaptane, methyl
                                     mercaptan, methylmercaptane,
                                     MERCAPTOMETHYLE, methylmercaptan,
                                     methylenethiol
     Autonom Name (AUN):             Methanethiol
     Lin. Struct. Formula (LSF):     HSCH3
     Molec. Formula (MF):            C H4 S
     Formula Weight (FW):            48.1088
     InChi Key: (INCHI):             LSDPWZHWYPCBBB-UHFFFAOYSA-N
     Alternate InChi Key: (AINCHI):  LSDPWZHWYPCBBB-UHFFFAOYAW
     Compound Type (CTYPE):          acyclic
     Markush Ref. Count (MARKREF):   5
     Entry Date (DED):               1989/02/27
     Update Date (DUPD):             2011/03/22
```

Field Availability:

Code	Name	Occurrence
AN	Accession Number	1
BPR	Basic Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	7
AUN	Autonomname	1
LSF	Linearized Structure Formula	1
MF	Molecular Formula	1
FW	Formula Weight	1
INCHI	InChi Key	1
AINCHI	Alternate InChi Key	1
CTYPE	Compound Type	1
MARKREF	Markush Reference Count	1
DED	Entry Date	1
DUPD	Update Date	1
ADSM	Adsorption (MCS)	45
ASSM	Association (MCS)	23
AZE	Azeotrope (MCS)	4
BIO	Biological Behaviour	2
BIOD	Biodegradation	17
BP	Boiling Point	11
CDER	Chemical Derivative	43
CNF	Conformation	2
COEV	Concentration in Environment	4
CP	Heat Capacity Cp	2
CP0	Heat Capacity Cp0	1
CRD	Critical Density	1
CRP	Critical Pressure	1
CRT	Critical Temperature	1
CRV	Critical Volume	1
CRYPH	Crystal Phase	2
CTP	Crystal Transition Point	1
DE	Dissociation Exponent	7
DEN	Density (Liquid)	7
DFM	Molecular Deformation	2
DIC	Dielectric Constant	1
DM	Dipole Moment	6
EBC	Energy Barrier of Conformation	1
ECDH	Abiotic Degradation, Hydrolysis	7
ECDP	Abiotic Degradation, Photolysis	2
ECTD	Ecological Mobility	4
ECTOX	Ecotoxicology	3
EDIS	Energy of Dissociation	10
ELCB	Electrochemical Behaviour	5
ELE	Electrical Data (MCS)	1
ENEM	Energy Data (MCS)	5
ESR	ESR Data	1
EXCA	Exposure Assessment	2
FINFO	Further Information	38
FLU	Fluorescence	1
GEO	Interatomic Distanc and Angle	6
GP	Gas Phase	1
HCOM	Enthalpy of Combustion	2
HFOR	Enthalpy of Formation	4
HFUS	Enthalpy of Fusion	1
HVAP	Enthalpy of Vaporization	2
INP	Isolation from Natural Product	9
IP	Ionization Potential	7
IR	Infrared Spectrum	28
LB	Substance Label	10
LIQPH	Liquid Phase	1
LLSM	Liquid/Liquid System (MCS)	2
LUM	Luminescence	1
LVSM	Liquid/Vapour System (MCS)	14

MEC	Mechanical Property	3
MECM	Mechanical & Physical Property (MCS)	2
MP	Melting Point	4
MS	Mass Spectrum	6
NMR	Nuclear Magnetic Resonance	16
OPT	Optics	1
OSM	Other Spectroscopic Methods	2
OTHE	Other Thermochemical Data	4
PHARM	Pharmacological Data	10
PHO	Phosphorescence	1
PSD	Patent Specific Data	6
RAS	Raman Spectrum	9
RI	Refractive Index	2
ROT	Rotational Spectrum	3
RSTR	Related Structure	5
SLB	Solubility (MCS)	3
SOLM	Solution Behaviour (MCS)	2
ST	Surface Tension	3
TRAM	Transport Phenomena (MCS)	1
USC	Use of Compound	6
UVS	UV and Visible Spectrum	9
VP	Vapour Pressure	7
XREF	Crossfile Reference	13
XS	Cross-Section	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	3074
RX.RAN	Reactant AN	2546
RX.PAN	Product AN	528

Vapour Pressure:

Value (VP) (bar)	Temp. (.T) (K)	Ref.	Note
1.5800257	293.15	1 2, 3	
0.8452655 - 2.7011837	274.55 - 307.05	4	1
0.0349397 - 1.7003755	215.25 - 293.15	5	2
0.5188892 - 1.4292118	263.15 - 288.15	6	
0.0548353 - 1.0141005	495.05 - 552.25	7	
0.7932659	273.15 - 469.95	8	

Reference(s):
1. Lestremau, Francois; Andersson, Fraes Annika T.; Desauziers, Valerie; Fanlo, Jean-Louis, Analytical Chemistry, CODEN: ANCHAM, 75(11), <2003>, 2626 - 2632
2. Wolff et al., Journal of Chemical Thermodynamics, CODEN: JCTDAF, 12, <1980>, 641,644, 645, 647, 650
3. Osborn; Scott, Journal of Chemical Thermodynamics, CODEN: JCTDAF, 12, <1980>, 429,434, 436
4. Osborn, A. G.; Scott, D. W., Journal of Chemical Thermodynamics, CODEN: JCTDAF, 12(5), <1980>, 429 - 438
5. Wolff, Hans; Szydlowski, Jerzy; Dill-Staffenberger, Ludmilla, Journal of Chemical Thermodynamics, CODEN: JCTDAF, 12(7), <1980>, 641 - 652
6. Jackowski, Andrzej W., Polish Journal of Chemistry, CODEN: PJCHDQ, 54(9), <1980>, 1765 - 1773
7. Russell; Osborne; Yost, Journal of the American Chemical Society, CODEN: JACSAT, 64, <1942>, 165
8. Berthoud; Brum, Journal de Chimie Physique et de Physico-Chimie Biologique, CODEN: JCPBAN, 21, <1924>, 144

Notes(s):
1. Table exists. Equation: Y

2. Table exists. Equation: lgp=-49087.2(K/T)E2-973.974(K/T)+6.12449

3.3 DETHERM ja CHEMSAFE

- **Joudutaan aina hakemaan komentokielellä, sillä ne eivät ole mukana STN Expressin automaattisissa toiminnossa.**
- **Poikkeavat rakenteeltaan ja hinnoittelultaan muista numeerisista tietokannoista. Jokainen taulukko on omana tietueenaan, joten yhdellä yhdisteellä voi olla paljon tietueita.**
- **Mukana myös seoksia.**
- **Yhdisteen haku**
  - **Hae aineet mieluiten Registryn tietuenumeron avulla. Voit myös hakea CAS:n rekisterinumeroilla perushakemistossa tai nimellä CN-kentästä**
  - **Rajoita joukkoa komponenttien lukumäärällä käyttämällä NC-kenttää (Number of Components) ja numeerisia operaattoreita (>, >=, =, <= ja <), sillä DETHERMissä on paljon monikomponenttisia seoksia**
- **Ominaisuuden haku**
  - **Ominaisuudet löytyvät nimillä ja koodeilla PROP-kentästä (Property)**
  - **Tarkastele PROP-kenttää EXPANDin avulla ja hae sitten sopivat ominaisuudet**
  - **Faasitasapainoja voit hakea myös STATE-kentän avulla:**
    - **tarkastele kenttää ensin EXPANDin avulla esim. E LIQUID-LIQUID EQUILIBRIUM/STATE**
- **Yhdistä AND-operaattorilla yhdiste ja ominaisuus eli rajoita haku niihin tietueisiin, joissa aineelle tai seokselle on annettu haluttu ominaisuus. Älä rajaa ominaisuustiedolla, jos**
  - **tietueita on suhteellisen vähän tai**
  - **olet kiinnostunut kaikista ominaisuuksista tai**
  - **et tiedä tarkkaan, mitä haluat.**
  - **Tulosta silloin kaikki löytyneet tietueet TRIAL-muodossa**
- **Tulostus**
  - **Taulukon hinta riippuu voimakkaasti taulukkorivien määrästä. Katso HELP COST. Jos kyseessä on kallis taulukko, kannattaa ensin tulostaa D BIB:illä lähteen bibliografiset tiedot ja hankkia lähdejulkaisu, jos se on helposti saatavissa .**
  - **Tulosta löytyneet tietueet aina ensin llmaisessa muodossa D TRIAL !!! <u>Älä tulosta heti D eikä D ALL!</u>**
  - **Tutki tulosteista systeemin ja ominaisuuksien tietoja**
  - **Kiinnitä huomiosi taulukkorivien määrään (ROW), sillä taulukon hinta riippuu siitä**
  - **Tulosta lopuksi ne tietueet kokonaan (D ALL), joissa on etsimäsi tiedot, ja joista olet valmis maksamaan täyden hinnan**
  - **Jos kyseessä on kallis taulukko, tulosta ensin D BIB:illä lähteen bibliografiset tiedot. Jos lähdejulkaisu on helposti saatavissa, voit hankkia sen itsellesi.**

```
=> FIL DETHERM
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FILE LAST UPDATED: 13 JAN 2010       <20100113/UP>
*********************************************************************
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*    CALCULATED FOR SET NOTICE ARE BASED ON THE HIGHEST PRICE       *
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=> S L1
L5          229 L1

=> S L5 AND NC=1
         341259 NC=1
L6          149 L5 AND NC=1

=> E VAPOR/FA
E1         79660     TI/FA
E2         79660     TITLE                          1/FA
E3             0 --> VAPOR/FA
E4        207353     VARIABLE RELATION              1/FA
E5        140814     VARIABLE RELATION              2/FA
E6         22799     VARIABLE RELATION              3/FA
E7         14452     VARIABLE RELATION              4/FA
E8           712     VARIABLE RELATION              5/FA
E9          2144     VARIABLE RELATION              6/FA
E10          264     VARIABLE RELATION              7/FA
E11          621     VARIABLE RELATION              8/FA
E12          262     VARIABLE RELATION              9/FA

=> E VAPOR/PROP
E1             2     VACT/PROP
E2           448     VANADIUM CONTENT/PROP
E3             0 --> VAPOR/PROP
E4            10     VAPOR FRACTION/PROP
E5        103944     VAPOR PRESSURE/PROP
E6            29     VAPOR PRESSURE - TEMPERATURE DERIVATIVE/PROP
E7            63     VC3/PROP
E8             6     VC4/PROP
E9             1     VC5/PROP
E10          811     VI2/PROP
E11         3538     VISCOSITY/PROP
E12          760     VITRINITE CONTENT/PROP

=> S L6 AND E5
         103944 "VAPOR PRESSURE"/PROP
L7           23 L6 AND "VAPOR PRESSURE"/PROP

=> HELP COST

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=> D TRIAL 1-23

L7   ANSWER 1 OF 23  DETHERM  COPYRIGHT 2012 DECHEMA/FIZC on STN
Accession Number (AN):        20-100963  DETHERM
                              System     : Methanethiol
                              Property   : boiling point
                              Property   : vapor pressure
                              Table lines: 5

L7   ANSWER 2 OF 23  DETHERM  COPYRIGHT 2012 DECHEMA/FIZC on STN
Accession Number (AN):        20-97484  DETHERM
                              System     : Methanethiol
                              Property   : boiling point
                              Property   : vapor pressure
                              Table lines: 5

L7   ANSWER 3 OF 23  DETHERM  COPYRIGHT 2012 DECHEMA/FIZC on STN
Accession Number (AN):        20-90456  DETHERM
                              System     : Methanethiol
                              Property   : boiling point
                              Property   : vapor pressure
                              Table lines: 2

L7   ANSWER 4 OF 23  DETHERM  COPYRIGHT 2012 DECHEMA/FIZC on STN
Accession Number (AN):        20-77338  DETHERM
                              System     : Methanethiol
                              Property   : boiling point
                              Property   : vapor pressure
                              Table lines: 3

L7   ANSWER 5 OF 23  DETHERM  COPYRIGHT 2012 DECHEMA/FIZC on STN
Accession Number (AN):        20-77124  DETHERM
                              System     : Methanethiol
                              Property   : boiling point
                              Property   : vapor pressure
                              Table lines: 8

L7   ANSWER 6 OF 23  DETHERM  COPYRIGHT 2012 DECHEMA/FIZC on STN
Accession Number (AN):        20-76998  DETHERM
                              System     : Methanethiol
                              Property   : boiling point
                              Property   : vapor pressure
                              Table lines: 8

L7   ANSWER 7 OF 23  DETHERM  COPYRIGHT 2012 DECHEMA/FIZC on STN
Accession Number (AN):        20-72009  DETHERM
                              System     : Methanethiol
                              Property   : boiling point
                              Property   : vapor pressure
                              Table lines: 10

L7   ANSWER 8 OF 23  DETHERM  COPYRIGHT 2012 DECHEMA/FIZC on STN
Accession Number (AN):        20-10876  DETHERM
                              System     : Methanethiol
                              Property   : boiling point
                              Property   : vapor pressure
                              Table lines: 54

                              ……..
```

=> **D ALL**
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L7 ANSWER 1 OF 23 DETHERM COPYRIGHT 2012 DECHEMA/FIZC on STN

Bibliography for Table Number: 20-100963 DDB PURE
Accession Number (AN): 19-15428 DETHERM Full-text
Related Acc. No. (RACC): Tables: 20-100961 - 20-100966
Title (TI): Measurement of VLE (Tpx or Tpxy data) for Hydrogen Sulfide + (Dimethylsulfide or Ethylmethylsulfide or Carbon Disulfide) and Methane Solubilities in (Dimethylsulfide or Ethylmethylsulfide or Methylmercaptan or Ethylmercaptan)
Author (AU): Guilbot, P.; Fischer, K.; Valtz, A.; Theveneau, P.; Baba-Ahmed, A.; Richon, D.
Source (SO): Report,(2007), 1-47
Document Type (DT): Report
Classification Code (CC): PRP: All properties (general)

Identification of System
System Description (SYST): O10 organic, pure compound
Substance (1) of (1):
Chemical Name (CN): Methanethiol
Synonyms: Methyl mercaptan; Mercaptomethane
Molecular Formula (MF): C H4 S
CAS Reg. Number (RN): 74-93-1

Data Information
Property (1) of (2):
Property (PROP): BP boiling point (boiling temperature, bubble temperature, temperature)
Original Unit: K
SI Unit : K
Data Type (DATA): experimental value
Desc. of State (STATE): vapor-liquid equilibrium; saturated condition

Property (2) of (2):
Property (PROP): VP vapor pressure
Original Unit: kPa
SI Unit : Pa
Data Type (DATA): experimental value
Desc. of State (STATE): vapor-liquid equilibrium; saturated condition

SI UNIT VALUES

1: BP (K)	2: VP (Pa)
243.19	2e+04
258.	4.2e+04
272.98	8e+04
293.35	1.7e+05
298.23	2e+05

Billing Class: 1

3.4 (H)CAplus

- **Tutki, jos jotakin ominaisuutta ei löydy numeerisesta tietokannoista.**
- **Hae yhdiste Registryssä saadun joukkonumeron avulla.**
- **Yhdistä se (S)-operaattorilla ominaisuuteen, jolloin ominaisuus on nimenomaan etsittävän yhdisteen määreenä samassa indeksitermissä.**
- **Tulosta ensin D SCAN tai D SCAN TI HITIND tai D SAM tai D TI HITIND**

```
=> FIL HCAPLUS
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USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE:  July 2012

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This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> S L1(S)((VAPOR OR VAPOUR)(S)PRESSURE)
          9242 L1
        690605 VAPOR
         80646 VAPORS
        737200 VAPOR
                 (VAPOR OR VAPORS)
                                  .....
       1765671 PRESSURE
                 (PRESSURE OR PRESSURES)
L8            8 L1(S)((VAPOR OR VAPOUR)(S)PRESSURE)



=> D TI HITIND 1-8
                                  .....

L8   ANSWER 6 OF 8  HCAPLUS  COPYRIGHT 2012 ACS on STN
TI   Vapor pressures of 17 miscellaneous organic compounds
CC   22-8 (Physical Organic Chemistry)
IT   74-93-1P, preparation   78-81-9P   100-41-4P, preparation
     100-53-8P   103-29-7P   106-88-7P   107-47-1P   151-56-4P, preparation
     259-79-0P   372-18-9P   503-30-0P   540-36-3P   765-30-0P   1067-20-5P
     1120-56-5P   4095-22-1P   21490-63-1P
     RL: PRP (Properties); PREP (Preparation)
        (vapor pressure of)
                                  .....
```

=> **D IBIB AB HITIND 6**

L10 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1942:9725 HCAPLUS Full-text
DOCUMENT NUMBER: 36:9725
ORIGINAL REFERENCE NO.: 36:1542a-c
TITLE: The heat capacity, entropy, heats of fusion, transition and vaporization and vapor pressures of methyl mercaptan
AUTHOR(S): Russell, Horace, Jr.; Osborne, Darrell W.; Yost, Don M.
SOURCE: Journal of the American Chemical Society (1942), 64, 165-9
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB The heat capacities of solid and liquid MeSH were measured over the temperature range 14-273°K. There is a slow isothermal transition at 137.6 ± 0.1°K. (0°C. = 273.16°K.), the heat of transition being 52.5 ± 0.5 cal./mole. The m. p. of pure MeSH is 150.16 ± 0.02°K., and the heat of fusion is 1411.4 ± 2.0 cal./mole. The vapor pressure was measured in the range 222-279°K., and can be accurately represented by the equation log10 pmm. = 18.2749 - (1769.05/T) - 3.70248 log10, T; the b. p. from this equation is 279.12°K. (5.96°C.). The directly measured heat of vaporization at the normal b. p. is 5872 ± 4 cal./mole. The entropy of MeSH at one atmospheric and 279.12°K. is 60.16 ± 0.10 cal./degree/mole for the ideal vapor. Comparison of this value with that calculated from mol. data leads to a barrier of 1460 ± 270 cal./mole restricting the rotation of the Me group.
CC 2 (General and Physical Chemistry)
IT 74-93-1, Methanethiol
(entropy, heat capacity, heats of fusion, transition and vaporization, and vapor pressure of)

=> **D HIS NOF**

FILE 'REGISTRY' ENTERED AT 12:18:02 ON 19 SEP 2012
E METHYL MERCAPTAN/CN
L1 1 SEA SPE=ON ABB=ON PLU=ON "METHYL MERCAPTAN"/CN
D
D FA
D VP

FILE 'REAXYSFILE' ENTERED AT 12:18:54 ON 19 SEP 2012
L2 3 SEA SPE=ON ABB=ON PLU=ON L1
E VAPOR/FA
L3 1 SEA SPE=ON ABB=ON PLU=ON L2 AND "VAPOUR PRESSURE"/FA
D

FILE 'DETHERM' ENTERED AT 12:23:03 ON 19 SEP 2012
L5 229 SEA SPE=ON ABB=ON PLU=ON L1
L6 149 SEA SPE=ON ABB=ON PLU=ON L5 AND NC=1
E VAPOR/PROP
L7 23 SEA SPE=ON ABB=ON PLU=ON L6 AND "VAPOR PRESSURE"/PROP
D TRIAL 1-23
D ALL

FILE 'HCAPLUS' ENTERED AT 12:24:21 ON 19 SEP 2012
L8 8 SEA SPE=ON ABB=ON PLU=ON L1(S)((VAPOR OR VAPOUR)(S)PRESSURE)

D TI HITIND 1-8