

1-Hexadecanethiol

Other names:	Cetyl mercaptan Hexadecanethiol Hexadecyl mercaptan hexadecane-1-thiol n-Hexadecanethiol n-Hexadecyl mercaptan
Inchi:	InChI=1S/C16H34S/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17/h17H,2-16H2,1H3
InchiKey:	ORTRWBYBJVGVQC-UHFFFAOYSA-N
Formula:	C16H34S
SMILES:	CCCCCCCCCCCCCCCCS
Mol. weight [g/mol]:	258.51
CAS:	2917-26-2

Physical Properties

Property code	Value	Unit	Source
gf	113.23	kJ/mol	Joback Method
hf	-335.09	kJ/mol	Joback Method
hfus	41.24	kJ/mol	Joback Method
hvap	57.95	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	6.398		Crippen Method
mcvol	252.650	ml/mol	McGowan Method
pc	1381.96	kPa	Joback Method
tb	628.34	K	Joback Method
tc	801.70	K	Joback Method
tf	306.54	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.30	J/mol×K	743.92	Joback Method
cpg	768.25	J/mol×K	772.81	Joback Method
cpg	680.62	J/mol×K	628.34	Joback Method

cpg	699.78	J/mol×K	657.23	Joback Method
cpg	718.09	J/mol×K	686.13	Joback Method
cpg	735.59	J/mol×K	715.02	Joback Method
cpg	783.47	J/mol×K	801.70	Joback Method
cpl	574.22	J/mol×K	300.00	NIST Webbook
hvapt	72.40	kJ/mol	556.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	460.70	K	0.90	NIST Webbook
tbrp	398.70	K	0.07	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.57330e+01
Coeff. B	-5.50148e+03
Coeff. C	-1.09940e+02
Temperature range (K), min.	466.13
Temperature range (K), max.	637.83

Sources

The Yaws Handbook of Vapor Pressure:
Crippen Method:

Crippen Method:

Joback Method:

McGowan Method:

NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

https://www.chemeo.com/doc/models/crippen_log10ws

https://en.wikipedia.org/wiki/Joback_method

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C2917262&Units=SI>

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvac:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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