1-Octadecanethiol

Other names:	1-Mercaptooctadecane
	Octadecanethiol
	Octadecyl mercaptan
	Stearyl mercaptan
	n-Octadecyl mercaptan
	octadecane-1-thiol
Inchi:	InChI=1S/C18H38S/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/h19H,2-18H2,1H
InchiKey:	QJAOYSPHSNGHNC-UHFFFAOYSA-N
Formula:	C18H38S
SMILES:	CCCCCCCCCCCCCCCCCCS
Mol. weight [g/mol]:	286.56
CAS:	2885-00-9

Physical Properties

Property code	Value	Unit	Source
gf	130.07	kJ/mol	Joback Method
hf	-376.37	kJ/mol	Joback Method
hfus	46.42	kJ/mol	Joback Method
hvap	62.40	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	7.178		Crippen Method
mcvol	280.830	ml/mol	McGowan Method
pc	1203.96	kPa	Joback Method
tb	674.10	K	Joback Method
tc	846.78	K	Joback Method
tf	329.08	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.68	J/mol×K	674.10	Joback Method
cpg	814.58	J/mol×K	702.88	Joback Method
cpg	833.59	J/mol×K	731.66	Joback Method

cpg	851.73	J/mol×K	760.44	Joback Method
cpg	869.05	J/mol×K	789.22	Joback Method
cpg	885.56	J/mol×K	818.00	Joback Method
cpg	901.30	J/mol×K	846.78	Joback Method
cpl	648.61	J/mol×K	300.00	NIST Webbook
hvapt	77.10	kJ/mol	581.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	480.20	K	1.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56517e+01
Coeff. B	-5.68104e+03
Coeff. C	-1.17168e+02
Temperature range (K), min.	486.93
Temperature range (K), max.	666.58

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2885009&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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
hvap:	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