Tetradecanethiol

Other names:	1-Mercaptotetradecane
	1-Tetradecanethiol
	Myristyl mercaptan
	Tetradecanethiol-(1)
	Tetradecyl mercaptan
	n-Tetradecyl mercaptan
	tetradecane-1-thiol
Inchi:	InChI=1S/C14H30S/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15/h15H,2-14H2,1H3
InchiKey:	GEKDEMKPCKTKEC-UHFFFAOYSA-N
Formula:	C14H30S
SMILES:	CCCCCCCCCCCCCCS
Mol. weight [g/mol]:	230.45
CAS:	2079-95-0

Physical Properties

Property code	Value	Unit	Source
gf	96.39	kJ/mol	Joback Method
hf	-293.81	kJ/mol	Joback Method
hfus	36.06	kJ/mol	Joback Method
hvap	53.50	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	5.617		Crippen Method
mcvol	224.470	ml/mol	McGowan Method
pc	1602.56	kPa	Joback Method
tb	582.58	K	Joback Method
tc	757.99	K	Joback Method
tf	284.00	K	Joback Method
vc	0.874	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.56	J/mol×K	728.76	Joback Method
cpg	571.84	J/mol×K	582.58	Joback Method

cpg	590.12	J/mol×K	611.82	Joback Method
cpg	607.61	J/mol×K	641.05	Joback Method
cpg	624.33	J/mol×K	670.29	Joback Method
cpg	640.31	J/mol×K	699.52	Joback Method
cpg	670.11	J/mol×K	757.99	Joback Method
cpl	501.57	J/mol×K	300.00	NIST Webbook
hvapt	67.30	kJ/mol	530.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58515e+01
Coeff. B	-5.31782e+03
Coeff. C	-1.02212e+02
Temperature range (K), min.	443.89
Temperature range (K), max.	606.75

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2079950&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

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

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

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume