3-Hexanethiol

Other names: 3-Mercaptohexane
hexane-3-thiol
Inchi: InChI=1S/C6H14S/c1-3-5-6(7)4-2/h6-7H,3-5H2,1-2H3
InchiKey: VOIGMFQJDZTEKW-UHFFFAOYSA-N
Formula: C6H14S
SMILES: CCCC(S)CC
Mol. weight [g/mol]: 118.24
CAS: 1633-90-5

Physical Properties

Property code	Value	Unit	Source
gf	26.59	kJ/mol	Joback Method
hf	-133.97	kJ/mol	Joback Method
hfus	11.81	kJ/mol	Joback Method
hvap	35.30	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.495		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
rinpol	862.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	850.00		NIST Webbook
ripol	1062.50		NIST Webbook
ripol	1058.00		NIST Webbook
ripol	1062.50		NIST Webbook
tb	399.10	K	Joback Method
tc	592.27	K	Joback Method
tf	178.84	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	204.79	J/mol×K	399.10	Joback Method
cpg	216.65	J/mol×K	431.30	Joback Method
cpg	228.00	J/mol×K	463.49	Joback Method
cpg	238.86	J/mol×K	495.69	Joback Method
cpg	249.24	J/mol×K	527.88	Joback Method
cpg	259.15	J/mol×K	560.08	Joback Method
cpg	268.61	J/mol×K	592.27	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41478e+01
Coeff. B	-3.51243e+03
Coeff. C	-5.54220e+01
Temperature range (K), min.	308.84
Temperature range (K), max.	452.92

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1633905&Units=SI

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

Legend

cpg: Ideal gas 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

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume