2-Hexanethiol

Other names: 2-Hexylthiol
Inchi: InChI=1S/C6H14S/c1-3-4-5-6(2)7/h6-7H,3-5H2,1-2H3
InchiKey: ABNPJVOPTXYSQW-UHFFFAOYSA-N
Formula: C6H14S
SMILES: CCCCC(C)S
Mol. weight [g/mol]: 118.24
CAS: 1679-06-7

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	850.00		NIST Webbook
rinpol	883.00		NIST Webbook
ripol	1066.30		NIST Webbook
ripol	1095.00		NIST Webbook
ripol	1062.10		NIST Webbook
tb	412.25 ± 0.20	K	NIST Webbook
tb	410.00 ± 6.00	K	NIST Webbook
tc	592.27	K	Joback Method
tf	126.20 ± 0.40	K	NIST Webbook
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.24	J/mol×K	527.88	Joback Method
cpg	259.15	J/mol×K	560.08	Joback Method

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	268.61	J/mol×K	592.27	Joback Method
hvapt	42.70	kJ/mol	375.00	NIST Webbook
hvapt	41.40	kJ/mol	375.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53950e+01
Coeff. B	-3.84241e+03
Coeff. C	-5.57000e+01
Temperature range (K), min.	310.04
Temperature range (K), max.	436.76

Sources

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

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

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1835

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1679067&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

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
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
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