1-Hexanol, 6-mercapto-

Other names: 6-Mercaptohexanol
Inchi: InChI=1S/C6H14OS/c7-5-3-1-2-4-6-8/h7-8H,1-6H2
InchiKey: UGZAJZLUKVKCBM-UHFFFAOYSA-N
Formula: C6H14OS
SMILES: OCCCCCCS
Mol. weight [g/mol]: 134.24
CAS: 1633-78-9

Physical Properties

Property code	Value	Unit	Source
gf	-107.79	kJ/mol	Joback Method
hf	-280.92	kJ/mol	Joback Method
hfus	19.43	kJ/mol	Joback Method
hvap	52.37	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	1.469		Crippen Method
mcvol	117.620	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
rinpol	1176.00		NIST Webbook
rinpol	1176.00		NIST Webbook
ripol	2100.00		NIST Webbook
ripol	2084.00		NIST Webbook
ripol	2100.00		NIST Webbook
tb	491.72	K	Joback Method
tc	672.12	K	Joback Method
tf	254.66	K	Joback Method
vc	0.445	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.96	J/mol×K	491.72	Joback Method
cpg	262.98	J/mol×K	521.79	Joback Method
cpg	272.57	J/mol×K	551.85	Joback Method

cpg	281.74	J/mol×K	581.92	Joback Method
cpg	290.51	J/mol×K	611.98	Joback Method
cpg	298.89	J/mol×K	642.05	Joback Method
cpg	306.88	J/mol×K	672.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1633789&Units=SI
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

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
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