3-Mercapto-1-hexanol

Inchi: InChI=1S/C6H14OS/c1-2-3-6(8)4-5-7/h6-8H,2-5H2,1H3
InchiKey: TYZFMFVWHZKYSE-UHFFFAOYSA-N
Formula: C6H14OS
SMILES: CCCC(S)CCO
Mol. weight [g/mol]: 134.24

Physical Properties

Property code	Value	Unit	Source
gf	-110.23	kJ/mol	Joback Method
hf	-286.20	kJ/mol	Joback Method
hfus	15.90	kJ/mol	Joback Method
hvap	51.98	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.467		Crippen Method
mcvol	117.620	ml/mol	McGowan Method
pc	3763.78	kPa	Joback Method
rinpol	1095.00		NIST Webbook
rinpol	1095.00		NIST Webbook
ripol	1847.00		NIST Webbook
ripol	1847.00		NIST Webbook
tb	491.28	K	Joback Method
tc	675.50	K	Joback Method
tf	239.66	K	Joback Method
vc	0.439	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.21	J/mol×K	491.28	Joback Method
cpg	263.51	J/mol×K	521.98	Joback Method
cpg	273.36	J/mol×K	552.69	Joback Method
cpg	282.76	J/mol×K	583.39	Joback Method
cpg	291.74	J/mol×K	614.09	Joback Method
cpg	300.30	J/mol×K	644.80	Joback Method

cpg	308.46	J/mol×K	675.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R602612&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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