3-Mercaptohexanol

Other names:	1-Hexanol, 3-mercapto-
	3-Mercapto-1-hexanol
	3-Mercaptohexan-1-ol
	3-Sulfanylhexan-1-ol
	3-Sulphanylhexan-1-ol
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
CAS:	51755-83-0

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	1126.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1125.00		NIST Webbook

rinpol	1127.00		NIST Webbook
rinpol	1095.00		NIST Webbook
ripol	1853.00		NIST Webbook
ripol	1825.00		NIST Webbook
ripol	1835.00		NIST Webbook
ripol	1871.00		NIST Webbook
ripol	1858.00		NIST Webbook
ripol	1853.00		NIST Webbook
ripol	1857.00		NIST Webbook
ripol	1853.00		NIST Webbook
ripol	1853.00		NIST Webbook
ripol	1853.00		NIST Webbook
ripol	1853.00		NIST Webbook
ripol	1853.00		NIST Webbook
ripol	1858.00		NIST Webbook
ripol	1836.00		NIST Webbook
ripol	1835.00		NIST Webbook
ripol	1835.00		NIST Webbook
ripol	1863.00		NIST Webbook
ripol	1835.00		NIST Webbook
ripol	1870.00		NIST Webbook
ripol	1875.00		NIST Webbook
ripol	1866.00		NIST Webbook
ripol	1872.00		NIST Webbook
ripol	1825.00		NIST Webbook
ripol	1857.00		NIST Webbook
ripol	1869.00		NIST Webbook
ripol	1836.00		NIST Webbook
ripol	1863.00		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

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=C51755830&Units=SI

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