3-Mercapto-2-methylbutanol

Inchi: InChI=1S/C5H12OS/c1-4(3-6)5(2)7/h4-7H,3H2,1-2H3
InchiKey: RFMHFOPFUZZBAD-UHFFFAOYSA-N
Formula: C5H12OS
SMILES: CC(S)C(C)CO
Mol. weight [g/mol]: 120.21

Physical Properties

Property code	Value	Unit	Source
gf	-121.09	kJ/mol	Joback Method
hf	-270.84	kJ/mol	Joback Method
hfus	9.79	kJ/mol	Joback Method
hvap	49.36	kJ/mol	Joback Method
log10ws	-1.12		Crippen Method
logp	0.933		Crippen Method
mcvol	103.530	ml/mol	McGowan Method
pc	4294.29	kPa	Joback Method
rinpol	987.00		NIST Webbook
rinpol	987.00		NIST Webbook
tb	467.96	K	Joback Method
tc	658.24	K	Joback Method
tf	213.39	K	Joback Method
vc	0.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.56	J/mol×K	467.96	Joback Method
cpg	222.02	J/mol×K	499.67	Joback Method
cpg	231.06	J/mol×K	531.39	Joback Method
cpg	239.68	J/mol×K	563.10	Joback Method
cpg	247.90	J/mol×K	594.82	Joback Method
cpg	255.72	J/mol×K	626.53	Joback Method
cpg	263.16	J/mol×K	658.24	Joback Method

Sources

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=R611691&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume