3-Mercapto-2-butylpropanol

Inchi: InChI=1S/C7H16OS/c1-2-3-4-7(5-8)6-9/h7-9H,2-6H2,1H3
InchiKey: BGYDAZPBSVHKRV-UHFFFAOYSA-N
Formula: C7H16OS
SMILES: CCCCC(CO)CS
Mol. weight [g/mol]: 148.27

Physical Properties

Property code	Value	Unit	Source
gf	-101.81	kJ/mol	Joback Method
hf	-306.84	kJ/mol	Joback Method
hfus	18.49	kJ/mol	Joback Method
hvap	54.20	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	1.715		Crippen Method
mcvol	131.710	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
rinpol	1218.00		NIST Webbook
rinpol	1218.00		NIST Webbook
rinpol	1218.00		NIST Webbook
ripol	1985.00		NIST Webbook
tb	514.16	K	Joback Method
tc	696.47	K	Joback Method
tf	250.93	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.10	J/mol×K	514.16	Joback Method
cpg	307.40	J/mol×K	544.54	Joback Method
cpg	318.20	J/mol×K	574.93	Joback Method
cpg	328.52	J/mol×K	605.31	Joback Method
cpg	338.36	J/mol×K	635.70	Joback Method
cpg	347.75	J/mol×K	666.08	Joback Method

cpg	356.70	J/mol×K	696.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R291975&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