3-Mercapto-2-methyl-1-pentanol, # 2

Inchi: InChI=1S/C6H14OS/c1-3-6(8)5(2)4-7/h5-8H,3-4H2,1-2H3
InchiKey: HABNNYNSJFKZFE-UHFFFAOYSA-N
Formula: C6H14OS
SMILES: CCC(S)C(C)CO
Mol. weight [g/mol]: 134.24

Physical Properties

Property code	Value	Unit	Source
gf	-112.67	kJ/mol	Joback Method
hf	-291.48	kJ/mol	Joback Method
hfus	12.38	kJ/mol	Joback Method
hvap	51.59	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.323		Crippen Method
mcvol	117.620	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
rinpol	1084.00		NIST Webbook
tb	490.84	K	Joback Method
tc	679.02	K	Joback Method
tf	224.66	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.45	J/mol×K	490.84	Joback Method
cpg	264.05	J/mol×K	522.20	Joback Method
cpg	274.16	J/mol×K	553.57	Joback Method
cpg	283.81	J/mol×K	584.93	Joback Method
cpg	293.00	J/mol×K	616.29	Joback Method
cpg	301.75	J/mol×K	647.66	Joback Method
cpg	310.08	J/mol×K	679.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R602934&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume