4-Mercapto-3-methylpentan-2-ol, # 1

Inchi: InChI=1S/C6H14OS/c1-4(5(2)7)6(3)8/h4-8H,1-3H3
InchiKey: IAEUQPZVOWVIES-UHFFFAOYSA-N
Formula: C6H14OS
SMILES: CC(O)C(C)C(C)S
Mol. weight [g/mol]: 134.24

Physical Properties

Property code	Value	Unit	Source
gf	-115.11	kJ/mol	Joback Method
hf	-296.76	kJ/mol	Joback Method
hfus	8.86	kJ/mol	Joback Method
hvap	51.20	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	1.322		Crippen Method
mcvol	117.620	ml/mol	McGowan Method
pc	3838.78	kPa	Joback Method
rinpol	1022.00		NIST Webbook
rinpol	1022.00		NIST Webbook
tb	490.40	K	Joback Method
tc	682.69	K	Joback Method
tf	209.66	K	Joback Method
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.69	J/mol×K	490.40	Joback Method
cpg	264.59	J/mol×K	522.45	Joback Method
cpg	274.99	J/mol×K	554.50	Joback Method
cpg	284.88	J/mol×K	586.54	Joback Method
cpg	294.29	J/mol×K	618.59	Joback Method
cpg	303.24	J/mol×K	650.64	Joback Method
cpg	311.73	J/mol×K	682.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R603046&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

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