4-Mercapto-4-methylpentan-2-ol

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

Physical Properties

Property code	Value	Unit	Source
gf	-107.39	kJ/mol	Joback Method
hf	-294.95	kJ/mol	Joback Method
hfus	8.49	kJ/mol	Joback Method
hvap	50.68	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.466		Crippen Method
mcvol	117.620	ml/mol	McGowan Method
pc	3853.09	kPa	Joback Method
rinpol	952.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	952.00		NIST Webbook
tb	488.05	K	Joback Method
tc	683.77	K	Joback Method
tf	242.08	K	Joback Method
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.48	J/mol×K	488.05	Joback Method
cpg	267.70	J/mol×K	520.67	Joback Method
cpg	278.28	J/mol×K	553.29	Joback Method
cpg	288.26	J/mol×K	585.91	Joback Method
cpg	297.65	J/mol×K	618.53	Joback Method
cpg	306.50	J/mol×K	651.15	Joback Method
cpg	314.83	J/mol×K	683.77	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=R602781&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume