3-Mercapto-2,2-dimethyl-1-propanol

Inchi: InChI=1S/C5H12OS/c1-5(2,3-6)4-7/h6-7H,3-4H2,1-2H3
InchiKey: YCCMKEDQXNVBHB-UHFFFAOYSA-N
Formula: C5H12OS
SMILES: CC(C)(CO)CS
Mol. weight [g/mol]: 120.21

Physical Properties

Property code	Value	Unit	Source
gf	-113.37	kJ/mol	Joback Method
hf	-269.03	kJ/mol	Joback Method
hfus	9.42	kJ/mol	Joback Method
hvap	48.84	kJ/mol	Joback Method
log10ws	-1.01		Crippen Method
logp	0.935		Crippen Method
mcvol	103.530	ml/mol	McGowan Method
pc	4311.22	kPa	Joback Method
rinpol	962.00		NIST Webbook
ripol	1680.00		NIST Webbook
tb	465.61	K	Joback Method
tc	659.33	K	Joback Method
tf	245.81	K	Joback Method
vc	0.378	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.31	J/mol×K	465.61	Joback Method
cpg	225.15	J/mol×K	497.90	Joback Method
cpg	234.43	J/mol×K	530.18	Joback Method
cpg	243.17	J/mol×K	562.47	Joback Method
cpg	251.41	J/mol×K	594.76	Joback Method
cpg	259.16	J/mol×K	627.05	Joback Method
cpg	266.46	J/mol×K	659.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R568740&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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