1-Mercapto-2-propanol

Other names: 1-mercaptopropan-2-ol
Inchi: InChI=1S/C3H8OS/c1-3(4)2-5/h3-5H,2H2,1H3
InchiKey: FETFXNFGOYOOSP-UHFFFAOYSA-N
Formula: C3H8OS
SMILES: CC(O)CS
Mol. weight [g/mol]: 92.16
CAS: 1068-47-9

Physical Properties

Property code	Value	Unit	Source
gf	-135.49	kJ/mol	Joback Method
hf	-224.28	kJ/mol	Joback Method
hfus	8.13	kJ/mol	Joback Method
hvap	45.30	kJ/mol	Joback Method
log10ws	-0.53		Crippen Method
logp	0.297		Crippen Method
mcvol	75.350	ml/mol	McGowan Method
pc	5552.58	kPa	Joback Method
rinpol	742.00		NIST Webbook
rinpol	761.00		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	742.00		NIST Webbook
ripol	1492.00		NIST Webbook
ripol	1425.00		NIST Webbook
ripol	1425.00		NIST Webbook
tb	422.64	K	Joback Method
tc	612.40	K	Joback Method
tf	205.85	K	Joback Method
vc	0.271	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.20	J/mol×K	422.64	Joback Method

cpg	143.76	J/mol×K	454.27	Joback Method
cpg	150.04	J/mol×K	485.89	Joback Method
cpg	156.04	J/mol×K	517.52	Joback Method
cpg	161.77	J/mol×K	549.14	Joback Method
cpg	167.24	J/mol×K	580.77	Joback Method
cpg	172.45	J/mol×K	612.40	Joback Method

Sources

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=C1068479&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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