2-Mercapto-1-propanol

Inchi: InChI=1S/C3H8OS/c1-3(5)2-4/h3-5H,2H2,1H3
InchiKey: QNNVICQPXUUBSN-UHFFFAOYSA-N
Formula: C3H8OS
SMILES: CC(S)CO
Mol. weight [g/mol]: 92.16

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	769.00		NIST Webbook
ripol	1485.00		NIST Webbook
ripol	1485.00		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:	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=R568720&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume