Propanoic acid, 3-mercapto-2-(mercaptomethyl)-

Other names: 3-Mercapto-2-[mercaptomethyl]propionic acid
Propionic acid, 3-mercapto-2-(mercaptomethyl)-
Inchi: InChI=1S/C4H8O2S2/c5-4(6)3(1-7)2-8/h3,7-8H,1-2H2,(H,5,6)
InchiKey: KRHAHEQEKNJCSD-UHFFFAOYSA-N
Formula: C4H8O2S2
SMILES: O=C(O)C(CS)CS
Mol. weight [g/mol]: 152.24
CAS: 7634-96-0

Physical Properties

Property code	Value	Unit	Source
gf	-226.60	kJ/mol	Joback Method
hf	-319.02	kJ/mol	Joback Method
hfus	16.36	kJ/mol	Joback Method
hvap	61.01	kJ/mol	Joback Method
log10ws	-0.50		Crippen Method
logp	0.547		Crippen Method
mcvol	107.360	ml/mol	McGowan Method
pc	5818.28	kPa	Joback Method
tb	562.25	K	Joback Method
tc	780.14	K	Joback Method
tf	303.51	K	Joback Method
vc	0.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.55	J/mol×K	562.25	Joback Method
cpg	228.98	J/mol×K	598.56	Joback Method
cpg	235.96	J/mol×K	634.88	Joback Method
cpg	242.51	J/mol×K	671.19	Joback Method
cpg	248.65	J/mol×K	707.51	Joback Method
cpg	254.39	J/mol×K	743.82	Joback Method
cpg	259.74	J/mol×K	780.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7634960&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume