3-Mercaptopropanal

Inchi: InChI=1S/C3H6OS/c4-2-1-3-5/h2,5H,1,3H2
InchiKey: BMYLOHDOJPEVOR-UHFFFAOYSA-N
Formula: C3H6OS
SMILES: O=CCCS
Mol. weight [g/mol]: 90.14

Physical Properties

Property code	Value	Unit	Source
gf	-95.75	kJ/mol	Joback Method
hf	-152.35	kJ/mol	Joback Method
hfus	9.86	kJ/mol	Joback Method
hvap	35.73	kJ/mol	Joback Method
log10ws	-0.43		Crippen Method
logp	0.505		Crippen Method
mcvol	71.050	ml/mol	McGowan Method
pc	5343.52	kPa	Joback Method
rinpol	756.00		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	756.00		NIST Webbook
tb	379.56	K	Joback Method
tc	580.52	K	Joback Method
tf	202.03	K	Joback Method
vc	0.275	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	115.98	J/mol×K	379.56	Joback Method
cpg	122.05	J/mol×K	413.05	Joback Method
cpg	127.84	J/mol×K	446.55	Joback Method
cpg	133.38	J/mol×K	480.04	Joback Method
cpg	138.65	J/mol×K	513.53	Joback Method
cpg	143.68	J/mol×K	547.02	Joback Method

cpg	148.46	J/mol×K	580.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R205617&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume