3-Mercaptopropanol

Inchi: InChI=1S/C3H8OS/c4-2-1-3-5/h4-5H,1-3H2
InchiKey: SHLSSLVZXJBVHE-UHFFFAOYSA-N
Formula: C3H8OS
SMILES: OCCCS
Mol. weight [g/mol]: 92.16

Physical Properties

Property code	Value	Unit	Source
gf	-133.05	kJ/mol	Joback Method
hf	-219.00	kJ/mol	Joback Method
hfus	11.66	kJ/mol	Joback Method
hvap	45.69	kJ/mol	Joback Method
log10ws	-0.41		Crippen Method
logp	0.299		Crippen Method
mcvol	75.350	ml/mol	McGowan Method
pc	5486.97	kPa	Joback Method
rinpol	852.00		NIST Webbook
rinpol	852.00		NIST Webbook
tb	423.08	K	Joback Method
tc	608.50	K	Joback Method
tf	220.85	K	Joback Method
vc	0.277	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.08	J/mol×K	423.08	Joback Method
cpg	143.40	J/mol×K	453.98	Joback Method
cpg	149.46	J/mol×K	484.89	Joback Method
cpg	155.26	J/mol×K	515.79	Joback Method
cpg	160.82	J/mol×K	546.69	Joback Method
cpg	166.13	J/mol×K	577.60	Joback Method
cpg	171.20	J/mol×K	608.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R611819&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume