3-mercaptooctanol

Inchi: InChI=1S/C8H18OS/c1-2-3-4-5-8(10)6-7-9/h8-10H,2-7H2,1H3
InchiKey: WKAXDMPFNOOFMS-UHFFFAOYSA-N
Formula: C8H18OS
SMILES: CCCCCC(S)CCO
Mol. weight [g/mol]: 162.29

Physical Properties

Property code	Value	Unit	Source
gf	-93.39	kJ/mol	Joback Method
hf	-327.48	kJ/mol	Joback Method
hfus	21.08	kJ/mol	Joback Method
hvap	56.43	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.248		Crippen Method
mcvol	145.800	ml/mol	McGowan Method
pc	3012.33	kPa	Joback Method
rinpol	1302.00		NIST Webbook
tb	537.04	K	Joback Method
tc	717.51	K	Joback Method
tf	262.20	K	Joback Method
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.92	J/mol×K	537.04	Joback Method
cpg	353.12	J/mol×K	567.12	Joback Method
cpg	364.77	J/mol×K	597.20	Joback Method
cpg	375.89	J/mol×K	627.28	Joback Method
cpg	386.51	J/mol×K	657.35	Joback Method
cpg	396.64	J/mol×K	687.43	Joback Method
cpg	406.29	J/mol×K	717.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R292052&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