8-Mercaptooctanol

Inchi: InChI=1S/C8H18OS/c9-7-5-3-1-2-4-6-8-10/h9-10H,1-8H2
InchiKey: XJTWZETUWHTBTG-UHFFFAOYSA-N
Formula: C8H18OS
SMILES: OCCCCCCCCS
Mol. weight [g/mol]: 162.29

Physical Properties

Property code	Value	Unit	Source
gf	-90.95	kJ/mol	Joback Method
hf	-322.20	kJ/mol	Joback Method
hfus	24.61	kJ/mol	Joback Method
hvap	56.82	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.249		Crippen Method
mcvol	145.800	ml/mol	McGowan Method
pc	2986.06	kPa	Joback Method
rinpol	1393.00		NIST Webbook
rinpol	1393.00		NIST Webbook
ripol	2150.00		NIST Webbook
tb	537.48	K	Joback Method
tc	714.51	K	Joback Method
tf	277.20	K	Joback Method
vc	0.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.61	J/mol×K	537.48	Joback Method
cpg	352.51	J/mol×K	566.98	Joback Method
cpg	363.89	J/mol×K	596.49	Joback Method
cpg	374.78	J/mol×K	625.99	Joback Method
cpg	385.19	J/mol×K	655.50	Joback Method
cpg	395.13	J/mol×K	685.00	Joback Method
cpg	404.61	J/mol×K	714.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R568795&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume