2-Mercaptocyclohexanol, # 1

Inchi: InChI=1S/C6H12OS/c7-5-3-1-2-4-6(5)8/h5-8H,1-4H2
InchiKey: KPJQEIHXBJFQDP-UHFFFAOYSA-N
Formula: C6H12OS
SMILES: OC1CCCCC1S
Mol. weight [g/mol]: 132.22

Physical Properties

Property code	Value	Unit	Source
gf	-91.05	kJ/mol	Joback Method
hf	-246.94	kJ/mol	Joback Method
hfus	12.33	kJ/mol	Joback Method
hvap	52.49	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	1.220		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	4652.99	kPa	Joback Method
rinpol	1085.00		NIST Webbook
rinpol	1085.00		NIST Webbook
tb	506.60	K	Joback Method
tc	723.10	K	Joback Method
tf	257.80	K	Joback Method
vc	0.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.75	J/mol×K	506.60	Joback Method
cpg	251.39	J/mol×K	542.68	Joback Method
cpg	264.28	J/mol×K	578.77	Joback Method
cpg	276.44	J/mol×K	614.85	Joback Method
cpg	287.87	J/mol×K	650.93	Joback Method
cpg	298.61	J/mol×K	687.02	Joback Method
cpg	308.66	J/mol×K	723.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R568819&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