Episulfide isomer 1

Inchi: InChI=1S/C5H7NOS/c6-2-1-4(7)5-3-8-5/h4-5,7H,1,3H2
InchiKey: YHHMEZJFUCZIOV-UHFFFAOYSA-N
Formula: C5H7NOS
SMILES: N#CCC(O)C1CS1
Mol. weight [g/mol]: 129.18

Physical Properties

Property code	Value	Unit	Source
gf	85.75	kJ/mol	Joback Method
hf	-21.10	kJ/mol	Joback Method
hfus	12.57	kJ/mol	Joback Method
hvap	59.22	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	0.376		Crippen Method
mcvol	94.050	ml/mol	McGowan Method
pc	4450.38	kPa	Joback Method
rinpol	1227.30		NIST Webbook
rinpol	1227.30		NIST Webbook
tb	562.19	K	Joback Method
tc	773.12	K	Joback Method
tf	358.31	K	Joback Method
vc	0.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.97	J/mol×K	562.19	Joback Method
cpg	219.41	J/mol×K	597.35	Joback Method
cpg	226.35	J/mol×K	632.50	Joback Method
cpg	232.83	J/mol×K	667.66	Joback Method
cpg	238.89	J/mol×K	702.81	Joback Method
cpg	244.57	J/mol×K	737.97	Joback Method
cpg	249.90	J/mol×K	773.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U414792&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