Cyclohexane, 1,2-bis-(methylthio), trans

Inchi: InChI=1S/C8H16S2/c1-9-7-5-3-4-6-8(7)10-2/h7-8H,3-6H2,1-2H3/t7-,8-/m1/s1
InchiKey: UOVDQPXIRFSKOV-HTQZYQBOSA-N
Formula: C8H16S2
SMILES: CSC1CCCCC1SC
Mol. weight [g/mol]: 176.34

Physical Properties

Property code	Value	Unit	Source
gf	99.46	kJ/mol	Joback Method
hf	-90.73	kJ/mol	Joback Method
hfus	17.64	kJ/mol	Joback Method
hvap	47.16	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	3.024		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
rinpol	1389.00		NIST Webbook
tb	534.88	K	Joback Method
tc	783.39	K	Joback Method
tf	251.86	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.38	J/mol×K	534.88	Joback Method
cpg	347.50	J/mol×K	576.30	Joback Method
cpg	365.44	J/mol×K	617.72	Joback Method
cpg	382.23	J/mol×K	659.13	Joback Method
cpg	397.87	J/mol×K	700.55	Joback Method
cpg	412.36	J/mol×K	741.97	Joback Method
cpg	425.70	J/mol×K	783.39	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R121732&Units=SI

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