Cyclohexane, 1-methyl-4-(1-methylethyl)-1,2-bis-(methylthio)

Inchi: InChI=1S/C12H24S2/c1-9(2)10-6-7-12(3,14-5)11(8-10)13-4/h9-11H,6-8H2,1-5H3/t10?,11

InchiKey: QZBLXHCJEOLPQK-PQDIPPBSSA-N

Formula: C12H24S2

SMILES: CSC1CC(C(C)C)CCC1(C)SC

Mol. weight [g/mol]: 232.45

Physical Properties

Property code	Value	Unit	Source
gf	117.50	kJ/mol	Joback Method
hf	-183.67	kJ/mol	Joback Method
hfus	19.25	kJ/mol	Joback Method
hvap	54.21	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	4.296		Crippen Method
mcvol	201.780	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
rinpol	1795.00		NIST Webbook
tb	621.53	K	Joback Method
tc	864.78	K	Joback Method
tf	301.60	K	Joback Method
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.96	J/mol×K	621.53	Joback Method
cpg	551.27	J/mol×K	662.07	Joback Method
cpg	572.24	J/mol×K	702.61	Joback Method
cpg	592.02	J/mol×K	743.16	Joback Method
cpg	610.73	J/mol×K	783.70	Joback Method
cpg	628.49	J/mol×K	824.24	Joback Method
cpg	645.45	J/mol×K	864.78	Joback Method

Sources

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=R121747&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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