Cyclohexane, trans-1-methyl-4-(1-methylethyl), 2,3-bis-(methylthio)

Inchi: InChI=1S/C12H24S2/c1-8(2)10-7-6-9(3)11(13-4)12(10)14-5/h8-12H,6-7H2,1-5H3/t9?,10

InchiKey: WYXMBTZBVVOMRW-QQFIATSDSA-N

Formula: C12H24S2

SMILES: CSC1C(C)CCC(C(C)C)C1SC

Mol. weight [g/mol]: 232.45

Physical Properties

Property code	Value	Unit	Source
gf	115.28	kJ/mol	Joback Method
hf	-219.25	kJ/mol	Joback Method
hfus	26.62	kJ/mol	Joback Method
hvap	55.05	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	4.152		Crippen Method
mcvol	201.780	ml/mol	McGowan Method
pc	2025.41	kPa	Joback Method
rinpol	1734.00		NIST Webbook
tb	616.62	K	Joback Method
tc	850.51	K	Joback Method
tf	273.46	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.85	J/mol×K	616.62	Joback Method
cpg	555.80	J/mol×K	655.60	Joback Method
cpg	577.33	J/mol×K	694.58	Joback Method
cpg	597.45	J/mol×K	733.57	Joback Method
cpg	616.16	J/mol×K	772.55	Joback Method
cpg	633.46	J/mol×K	811.53	Joback Method
cpg	649.35	J/mol×K	850.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R121767&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