Bicyclo[3.3.1]heptane, 6,6-dimethyl-2,7-bis-(methylthio)

Inchi: InChI=1S/C12H22S2/c1-11(2)9-5-6-12(14-4,8-13-3)10(11)7-9/h9-10H,5-8H2,1-4H3

InchiKey: BAFXWEACXKZZCP-UHFFFAOYSA-N

Formula: C12H22S2

SMILES: CSCC1(SC)CCC2CC1C2(C)C

Mol. weight [g/mol]: 230.43

Physical Properties

Property code	Value	Unit	Source
gf	199.40	kJ/mol	Joback Method
hf	-78.03	kJ/mol	Joback Method
hfus	18.81	kJ/mol	Joback Method
hvap	53.02	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.907		Crippen Method
mcvol	190.920	ml/mol	McGowan Method
pc	2433.84	kPa	Joback Method
rinpol	1690.00		NIST Webbook
rinpol	1690.00		NIST Webbook
tb	620.41	K	Joback Method
tc	868.89	K	Joback Method
tf	365.48	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.00	J/mol×K	620.41	Joback Method
cpg	528.34	J/mol×K	661.82	Joback Method
cpg	547.52	J/mol×K	703.24	Joback Method
cpg	565.87	J/mol×K	744.65	Joback Method
cpg	583.73	J/mol×K	786.07	Joback Method
cpg	601.43	J/mol×K	827.48	Joback Method
cpg	619.30	J/mol×K	868.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R121698&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