Bicyclo[3.1.1]heptane, 2,6,6-trimethyl, 2,3-bis-(methylthio)

Inchi: InChI=1S/C12H22S2/c1-11(2)8-6-9(11)12(3,14-5)10(7-8)13-4/h8-10H,6-7H2,1-5H3/t8?,9

InchiKey: VGISVROEVMZEBM-GZJRGEOXSA-N

Formula: C12H22S2

SMILES: CSC1CC2CC(C2(C)C)C1(C)SC

Mol. weight [g/mol]: 230.43

Physical Properties

Property code	Value	Unit	Source
gf	191.69	kJ/mol	Joback Method
hf	-98.37	kJ/mol	Joback Method
hfus	19.88	kJ/mol	Joback Method
hvap	52.71	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.906		Crippen Method
mcvol	190.920	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinpol	1670.00		NIST Webbook
rinpol	1670.00		NIST Webbook
tb	615.74	K	Joback Method
tc	864.38	K	Joback Method
tf	361.24	K	Joback Method
vc	0.715	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.67	J/mol×K	615.74	Joback Method
cpg	530.58	J/mol×K	657.18	Joback Method
cpg	550.29	J/mol×K	698.62	Joback Method
cpg	569.12	J/mol×K	740.06	Joback Method
cpg	587.40	J/mol×K	781.50	Joback Method
cpg	605.43	J/mol×K	822.94	Joback Method
cpg	623.56	J/mol×K	864.38	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=R121683&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

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