2,3-Dimethyl-5,6-dithiabicyclo[2.1.1]hexane, 5,5-dioxide

Inchi: InChI=1S/C6H10O2S2/c1-3-4(2)6-9-5(3)10(6,7)8/h3-6H,1-2H3
InchiKey: KXXBBGPZYBPBEO-UHFFFAOYSA-N
Formula: C6H10O2S2
SMILES: CC1C(C)C2SC1S2(=O)=O
Mol. weight [g/mol]: 178.27

Physical Properties

Property code	Value	Unit	Source
gf	-316.22	kJ/mol	Joback Method
hf	-466.95	kJ/mol	Joback Method
hfus	24.27	kJ/mol	Joback Method
hvap	51.60	kJ/mol	Joback Method
log10ws	-1.57		Crippen Method
logp	1.086		Crippen Method
mcvol	118.120	ml/mol	McGowan Method
pc	4602.62	kPa	Joback Method
rinpol	1421.00		NIST Webbook
tb	415.48	K	Joback Method
tc	613.16	K	Joback Method
tf	355.84	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.18	J/mol×K	415.48	Joback Method
cpg	252.59	J/mol×K	448.43	Joback Method
cpg	266.14	J/mol×K	481.37	Joback Method
cpg	278.88	J/mol×K	514.32	Joback Method
cpg	290.82	J/mol×K	547.27	Joback Method
cpg	302.03	J/mol×K	580.21	Joback Method
cpg	312.54	J/mol×K	613.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U322303&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

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