Isoprothiolane sulfoxide

Inchi: InChI=1S/C12H18O5S2/c1-7(2)16-10(13)9(11(14)17-8(3)4)12-18-5-6-19(12)15/h7-8H,5-
InchiKey: ZFQQZUBSEINSSR-UHFFFAOYSA-N
Formula: C12H18O5S2
SMILES: CC(C)OC(=O)C(C(=O)OC(C)C)=C1SCCS1=O
Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
gf	-512.50	kJ/mol	Joback Method
hf	-801.20	kJ/mol	Joback Method
hfus	28.18	kJ/mol	Joback Method
hvap	78.81	kJ/mol	Joback Method
log10ws	-2.05		Crippen Method
logp	1.597		Crippen Method
mcvol	218.230	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
rinpol	2193.00		NIST Webbook
tb	737.29	K	Joback Method
tc	959.29	K	Joback Method
tf	519.84	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.48	J/mol×K	737.29	Joback Method
cpg	604.91	J/mol×K	774.29	Joback Method
cpg	618.27	J/mol×K	811.29	Joback Method
cpg	630.61	J/mol×K	848.29	Joback Method
cpg	641.94	J/mol×K	885.29	Joback Method
cpg	652.29	J/mol×K	922.29	Joback Method
cpg	661.67	J/mol×K	959.29	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=R543429&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