2-Methylthianaphthene-1,1 dioxide

Other names: Benzo[b]thiophene 1,1-dioxide,2-methyl-
2-Methyl-benzo(b)thiophene-1,1-dioxide
Benzo[b]thiophene, 2-methyl-, 1,1-dioxide
Inchi: InChI=1S/C9H8O2S/c1-7-6-8-4-2-3-5-9(8)12(7,10)11/h2-6H,1H3
InchiKey: BRNMIIDEQOJZTP-UHFFFAOYSA-N
Formula: C9H8O2S
SMILES: CC1=Cc2ccccc2S1(=O)=O
Mol. weight [g/mol]: 180.22
CAS: 6224-55-1

Physical Properties

Property code	Value	Unit	Source
gf	-245.33	kJ/mol	Joback Method
hf	-314.54	kJ/mol	Joback Method
hfus	21.52	kJ/mol	Joback Method
hvap	57.37	kJ/mol	Joback Method
ie	9.10	eV	NIST Webbook
log10ws	-2.38		Crippen Method
logp	1.835		Crippen Method
mcvol	126.840	ml/mol	McGowan Method
pc	4756.24	kPa	Joback Method
tb	479.36	K	Joback Method
tc	693.23	K	Joback Method
tf	353.20	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.35	J/mol×K	479.36	Joback Method
cpg	266.87	J/mol×K	515.00	Joback Method
cpg	278.51	J/mol×K	550.65	Joback Method
cpg	289.32	J/mol×K	586.29	Joback Method
cpg	299.35	J/mol×K	621.94	Joback Method

cpg	308.63	J/mol×K	657.58	Joback Method
cpg	317.23	J/mol×K	693.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6224551&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume