Benzo[b]thiophene 1,1-dioxide, 3-methyl-

Other names:	3-Methyl-1-thiaindene 1,1-dioxide
	3-Methyl-benzo(b)thiophene-1,1-dioxide
	3-Methylbenzo[b]thiophene dioxide
	3-Methylbenzothiophene 1,1-dioxide
	Benzo[b]thiophene, 3-methyl-, 1,1-dioxide
Inchi:	InChI=1S/C9H8O2S/c1-7-6-12(10,11)9-5-3-2-4-8(7)9/h2-6H,1H3
InchiKey:	DCAZNDCIMXHKOS-UHFFFAOYSA-N
Formula:	C9H8O2S
SMILES:	CC1=CS(=O)(=O)c2ccccc21
Mol. weight [g/mol]:	180.22
CAS:	6406-91-3

Physical Properties

Property code	Value	Unit	Source
chl	-5196.00 ± 83.00	kJ/mol	NIST Webbook
gf	-245.33	kJ/mol	Joback Method
hf	-314.54	kJ/mol	Joback Method
hfl	214.00	kJ/mol	NIST Webbook
hfus	21.52	kJ/mol	Joback Method
hvap	57.37	kJ/mol	Joback Method
ie	9.20	eV	NIST Webbook
log10ws	-2.67		Aqueous Solubility Prediction 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=C6406913&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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

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