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]: 180.23

Physical Properties

Property code	Value	Unit	Source
hfus	21.52	kJ/mol	Joback Method
ie	9.10	eV	NIST Webbook
log10ws	-3.04		Cheméo Relay (1.0)
logp	1.835		Crippen Method
mcvol	126.840	ml/mol	McGowan 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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6224551&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume