Benzo[b]thiophene, 1,1-dioxide

Other names: Benzothiophene 1,1-dioxide
Thianaphthene 1,1-dioxide
Inchi: InChI=1S/C8H6O2S/c9-11(10)6-5-7-3-1-2-4-8(7)11/h1-6H
InchiKey: FRJNKYGTHPUSJR-UHFFFAOYSA-N
Formula: C8H6O2S
SMILES: O=S1(=O)C=Cc2ccccc21
Mol. weight [g/mol]: 166.20
CAS: 825-44-5

Physical Properties

Property code	Value	Unit	Source
gf	-244.12	kJ/mol	Joback Method
hf	-282.43	kJ/mol	Joback Method
hfus	19.32	kJ/mol	Joback Method
hvap	54.48	kJ/mol	Joback Method
ie	9.32	eV	NIST Webbook
ie	9.10	eV	NIST Webbook
log10ws	-1.96		Crippen Method
logp	1.445		Crippen Method
mcvol	112.750	ml/mol	McGowan Method
pc	5577.49	kPa	Joback Method
tb	451.50	K	Joback Method
tc	667.13	K	Joback Method
tf	329.41	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.11	J/mol×K	451.50	Joback Method
cpg	225.07	J/mol×K	487.44	Joback Method
cpg	236.11	J/mol×K	523.38	Joback Method
cpg	246.28	J/mol×K	559.31	Joback Method
cpg	255.64	J/mol×K	595.25	Joback Method

cpg	264.25	J/mol×K	631.19	Joback Method
cpg	272.15	J/mol×K	667.13	Joback Method

Sources

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=C825445&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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