Dibenzothiophene, 5-oxide

Other names: Dibenzothiophene sulfoxide
Dibenzothiophene S-oxide
Inchi: InChI=1S/C12H8OS/c13-14-11-7-3-1-5-9(11)10-6-2-4-8-12(10)14/h1-8H
InchiKey: NGDPCAMPVQYGCW-UHFFFAOYSA-N
Formula: C12H8OS
SMILES: O=S1c2ccccc2-c2ccccc21
Mol. weight [g/mol]: 200.26
CAS: 1013-23-6

Physical Properties

Property code	Value	Unit	Source
gf	137.41	kJ/mol	Joback Method
hf	62.22	kJ/mol	Joback Method
hfus	22.69	kJ/mol	Joback Method
hvap	59.78	kJ/mol	Joback Method
ie	8.10	eV	NIST Webbook
ie	8.43	eV	NIST Webbook
log10ws	-3.49		Crippen Method
logp	2.834		Crippen Method
mcvol	143.780	ml/mol	McGowan Method
pc	4098.62	kPa	Joback Method
tb	577.48	K	Joback Method
tc	826.37	K	Joback Method
tf	417.63	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.52	J/mol×K	577.48	Joback Method
cpg	331.67	J/mol×K	618.96	Joback Method
cpg	343.60	J/mol×K	660.44	Joback Method
cpg	354.44	J/mol×K	701.93	Joback Method
cpg	364.34	J/mol×K	743.41	Joback Method

cpg	373.41	J/mol×K	784.89	Joback Method
cpg	381.80	J/mol×K	826.37	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=C1013236&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