2-Bromobenzothiophene sulfone

Other names:	2-Bromothianaphthene 1,1-dioxide
	2-Bromo-benzo(b)thiophene-1,1-dioxide
	Benzo[b]thiophene, 2-bromo-, 1,1-dioxide
	2-Bromobenzothiophene 1,1-dioxide
Inchi:	InChI=1S/C8H5BrO2S/c9-8-5-6-3-1-2-4-7(6)12(8,10)11/h1-5H
InchiKey:	GSNSVTOQAJSJSG-UHFFFAOYSA-N
Formula:	C8H5BrO2S
SMILES:	O=S1(=O)C(Br)=Cc2ccccc21
Mol. weight [g/mol]:	245.09
CAS:	5350-05-0

Physical Properties

Property code	Value	Unit	Source
gf	-239.43	kJ/mol	Joback Method
hf	-267.57	kJ/mol	Joback Method
hfus	24.22	kJ/mol	Joback Method
hvap	61.58	kJ/mol	Joback Method
ie	9.10	eV	NIST Webbook
log10ws	-2.89		Crippen Method
logp	2.167		Crippen Method
mcvol	130.250	ml/mol	McGowan Method
pc	6056.11	kPa	Joback Method
tb	522.64	K	Joback Method
tc	756.44	K	Joback Method
tf	401.73	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.37	J/mol×K	522.64	Joback Method
cpg	257.68	J/mol×K	561.61	Joback Method
cpg	267.08	J/mol×K	600.57	Joback Method
cpg	275.64	J/mol×K	639.54	Joback Method

cpg	283.42	J/mol×K	678.50	Joback Method
cpg	290.49	J/mol×K	717.47	Joback Method
cpg	296.94	J/mol×K	756.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5350050&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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