4-Bromophenyl sulfone

Other names:	Benzene, 1,1'-sulfonylbis(4-bromo-
	Bis(p-bromophenyl) sulfone
	Sulfone, bis(p-bromophenyl)
	4,4'-Dibromodiphenyl sulfone
Inchi:	InChI=1S/C12H8Br2O2S/c13-9-1-5-11(6-2-9)17(15,16)12-7-3-10(14)4-8-12/h1-8H
InchiKey:	QBNABJXQGRVIRA-UHFFFAOYSA-N
Formula:	C12H8Br2O2S
SMILES:	O=S(=O)(c1ccc(Br)cc1)c1ccc(Br)cc1
Mol. weight [g/mol]:	376.06
CAS:	2050-48-8

Physical Properties

Property code	Value	Unit	Source
gf	-184.18	kJ/mol	Joback Method
hf	-241.58	kJ/mol	Joback Method
hfus	36.09	kJ/mol	Joback Method
hvap	79.69	kJ/mol	Joback Method
ie	8.84 ± 0.05	eV	NIST Webbook
log10ws	-5.16		Crippen Method
logp	4.044		Crippen Method
mcvol	195.510	ml/mol	McGowan Method
pc	4789.21	kPa	Joback Method
tb	717.38	K	Joback Method
tc	981.11	K	Joback Method
tf	461.04	K	Joback Method
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.59	J/mol×K	717.38	Joback Method
cpg	439.23	J/mol×K	761.34	Joback Method
cpg	449.63	J/mol×K	805.29	Joback Method
cpg	458.87	J/mol×K	849.25	Joback Method

cpg	467.01	J/mol×K	893.20	Joback Method
cpg	474.13	J/mol×K	937.16	Joback Method
cpg	480.29	J/mol×K	981.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2050488&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

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