4-Bromobenzenesulphonamide

Other names: p-Bromobenzenesulfonamide
Benzenesulfonamide, p-bromo-
Benzenesulfonamide, 4-bromo-
Inchi: InChI=1S/C6H6BrNO2S/c7-5-1-3-6(4-2-5)11(8,9)10/h1-4H,(H2,8,9,10)
InchiKey: STYQHICBPYRHQK-UHFFFAOYSA-N
Formula: C6H6BrNO2S
SMILES: NS(=O)(=O)c1ccc(Br)cc1
Mol. weight [g/mol]: 236.09

Physical Properties

Property code	Value	Unit	Source
hfus	26.81	kJ/mol	Joback Method
ie	9.32	eV	Cheméo Relay (1.0)
log10ws	-2.87		Cheméo Relay (1.0)
logp	1.097		Crippen Method
mcvol	127.210	ml/mol	McGowan Method
tb	584.16	K	Cheméo Relay (1.0)
tf	429.97	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.52	J/mol×K	554.81	Joback Method
cpg	261.40	J/mol×K	594.60	Joback Method
cpg	270.52	J/mol×K	634.39	Joback Method
cpg	278.89	J/mol×K	674.18	Joback Method
cpg	286.54	J/mol×K	713.96	Joback Method
cpg	293.48	J/mol×K	753.75	Joback Method
cpg	299.72	J/mol×K	793.54	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C701348&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point