

4-Bromobenzenesulfonamide

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
CAS:	701-34-8

Physical Properties

Property code	Value	Unit	Source
gf	-285.35	kJ/mol	Joback Method
hf	-335.34	kJ/mol	Joback Method
hfus	26.81	kJ/mol	Joback Method
hvap	67.60	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	1.097		Crippen Method
mcvol	127.210	ml/mol	McGowan Method
pc	6979.30	kPa	Joback Method
tb	554.81	K	Joback Method
tc	793.54	K	Joback Method
tf	377.94	K	Joback Method
vc	0.480	m3/kmol	Joback Method

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

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=C701348&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
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

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