2-Bromobenzenesulfonyl chloride

Other names: Benzenesulfonyl chloride, 2-bromo-
Inchi: InChI=1S/C6H4BrClO2S/c7-5-3-1-2-4-6(5)11(8,9)10/h1-4H
InchiKey: VFPWGZNNRSQPBT-UHFFFAOYSA-N
Formula: C6H4BrClO2S
SMILES: O=S(=O)(Cl)c1ccccc1Br
Mol. weight [g/mol]: 255.52
CAS: 2905-25-1

Physical Properties

Property code	Value	Unit	Source
gf	-363.73	kJ/mol	Joback Method
hf	-384.87	kJ/mol	Joback Method
hfus	25.81	kJ/mol	Joback Method
hvap	61.34	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.377		Crippen Method
mcvol	129.470	ml/mol	McGowan Method
pc	5999.95	kPa	Joback Method
tb	519.71	K	Joback Method
tc	753.75	K	Joback Method
tf	324.60	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.86	J/mol×K	519.71	Joback Method
cpg	234.97	J/mol×K	558.72	Joback Method
cpg	243.40	J/mol×K	597.72	Joback Method
cpg	251.16	J/mol×K	636.73	Joback Method
cpg	258.26	J/mol×K	675.74	Joback Method
cpg	264.72	J/mol×K	714.74	Joback Method
cpg	270.56	J/mol×K	753.75	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2905251&Units=SI

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