5-Bromo-2-methoxybenzenesulphonyl chloride

Inchi: InChI=1S/C7H6BrClO3S/c1-12-6-3-2-5(8)4-7(6)13(9,10)11/h2-4H,1H3
InchiKey: IXSBNNRUQYYMRM-UHFFFAOYSA-N
Formula: C7H6BrClO3S
SMILES: COc1ccc(Br)cc1S(=O)(=O)Cl
Mol. weight [g/mol]: 285.55

Physical Properties

Property code	Value	Unit	Source
hfus	29.20	kJ/mol	Joback Method
logp	2.385		Crippen Method
mcvol	149.430	ml/mol	McGowan Method
tb	587.89	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.20	J/mol×K	569.99	Joback Method
cpg	298.02	J/mol×K	607.94	Joback Method
cpg	307.21	J/mol×K	645.90	Joback Method
cpg	315.75	J/mol×K	683.85	Joback Method
cpg	323.65	J/mol×K	721.80	Joback Method
cpg	330.90	J/mol×K	759.76	Joback Method
cpg	337.47	J/mol×K	797.71	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C23095058&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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature