

# 5-Bromo-2-methoxybenzenesulfonyl chloride

<b>Inchi:</b>	InChI=1S/C7H6BrClO3S/c1-12-6-3-2-5(8)4-7(6)13(9,10)11/h2-4H,1H3
<b>InchiKey:</b>	IXSBNNRUQYYMRM-UHFFFAOYSA-N
<b>Formula:</b>	C7H6BrClO3S
<b>SMILES:</b>	<chem>COc1ccc(Br)cc1S(=O)(=O)Cl</chem>
<b>Mol. weight [g/mol]:</b>	285.54
<b>CAS:</b>	23095-05-8

## Physical Properties

Property code	Value	Unit	Source
gf	-469.94	kJ/mol	Joback Method
hf	-549.20	kJ/mol	Joback Method
hfus	29.20	kJ/mol	Joback Method
hvap	66.64	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.385		Crippen Method
mcvol	149.430	ml/mol	McGowan Method
pc	4966.33	kPa	Joback Method
tb	569.99	K	Joback Method
tc	797.71	K	Joback Method
tf	370.62	K	Joback Method
vc	0.575	m3/kmol	Joback Method

## Temperature Dependent Properties

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

# Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C23095058&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C23095058&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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