

5-Bromo-2-chlorothiophene

Other names:	2-Chloro-5-bromothiophene 2-Bromo-5-chlorothiophene Thiophene, 2-bromo-5-chloro-
Inchi:	InChI=1S/C4H2BrClS/c5-3-1-2-4(6)7-3/h1-2H
InchiKey:	ZFAJPWYXLYGUJU-UHFFFAOYSA-N
Formula:	C4H2BrClS
SMILES:	Clc1ccc(Br)s1
Mol. weight [g/mol]:	197.48
CAS:	2873-18-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.08		Crippen Method
logp	3.164		Crippen Method
mcvol	93.850	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	343.20	K	2.40	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2873189&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

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