

5-Bromofuroic acid

Other names:	5-Bromo-2-furoic acid 5-Bromo furan-2-carboxylic acid 2-Furancarboxylic acid, 5-bromo- 2-Furoic acid, 5-bromo- 5-bromo-2-furanecarboxylic acid
Inchi:	InChI=1S/C5H3BrO3/c6-4-2-1-3(9-4)5(7)8/h1-2H,(H,7,8)
InchiKey:	YVTQHZDUDUCGRD-UHFFFAOYSA-N
Formula:	C5H3BrO3
SMILES:	O=C(O)c1ccc(Br)o1
Mol. weight [g/mol]:	190.98
CAS:	585-70-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.43		Crippen Method
logp	1.740		Crippen Method
mcvol	92.660	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C585706&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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