

2-Bromopyrimidine

Other names:	Pyrimidine, 2-bromo-
Inchi:	InChI=1S/C4H3BrN2/c5-4-6-2-1-3-7-4/h1-3H
InchiKey:	PGFIHORVILKHIA-UHFFFAOYSA-N
Formula:	C4H3BrN2
SMILES:	Brc1ncccn1
Mol. weight [g/mol]:	158.98
CAS:	4595-60-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.17		Crippen Method
logp	1.239		Crippen Method
mcvol	80.920	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4595602&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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<https://www.chemeo.com/cid/68-247-3/2-Bromopyrimidine.pdf>

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