

3-Bromochromone

Inchi:	InChI=1S/C9H5BrO2/c10-7-5-12-8-4-2-1-3-6(8)9(7)11/h1-5H
InchiKey:	IQIGYNPOESZBDJ-UHFFFAOYSA-N
Formula:	C9H5BrO2
SMILES:	O=c1c(Br)coc2ccccc12
Mol. weight [g/mol]:	225.04
CAS:	49619-82-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.60		Crippen Method
logp	2.555		Crippen Method
mcvol	123.690	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=C49619821&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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<https://www.chemeo.com/cid/54-540-2/3-Bromochromone.pdf>

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