

Quinoline, 6-methoxy-2-methyl-

Other names:	Quinaldine, 6-methoxy- 2-Methyl-6-methoxyquinoline 6-Methoxy-2-methylquinoline 6-Methoxyquinaldine
Inchi:	InChI=1S/C11H11NO/c1-8-3-4-9-7-10(13-2)5-6-11(9)12-8/h3-7H,1-2H3
InchiKey:	NAGJQQFMJKMXJQ-UHFFFAOYSA-N
Formula:	C11H11NO
SMILES:	<chem>COc1ccc2nc(C)ccc2c1</chem>
Mol. weight [g/mol]:	173.21
CAS:	1078-28-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.64		Crippen Method
logp	2.552		Crippen Method
mcvol	138.480	ml/mol	McGowan Method
rinpol	1514.00		NIST Webbook
rinpol	1514.00		NIST Webbook
tf	340.00 ± 3.00	K	NIST Webbook

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=C1078280&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
rinpol: Non-polar retention indices
tf: Normal melting (fusion) point

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