

Quinoline, 2,3,4-trimethyl-

Other names:	2,3,4-Trimethylquinoline
Inchi:	InChI=1S/C12H13N/c1-8-9(2)11-6-4-5-7-12(11)13-10(8)3/h4-7H,1-3H3
InchiKey:	VBCFHWSPNHEYGE-UHFFFAOYSA-N
Formula:	C12H13N
SMILES:	<chem>Cc1nc2ccccc2c(C)c1C</chem>
Mol. weight [g/mol]:	171.24
CAS:	2437-72-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.47		Crippen Method
logp	3.160		Crippen Method
mcvol	146.700	ml/mol	McGowan Method
rinpola	1616.00		NIST Webbook
tb	536.00 ± 4.00	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=C2437721&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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<https://www.chemeo.com/cid/14-428-1/Quinoline-2-3-4-trimethyl.pdf>

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