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: Cc1nc2ccccc2c(C)c1C
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
rinpol	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/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature