3,5-dimethylquinoline

Inchi: InChI=1S/C11H11N/c1-8-6-10-9(2)4-3-5-11(10)12-7-8/h3-7H,1-2H3
InchiKey: JOAWUJDFFAMORU-UHFFFAOYSA-N
Formula: C11H11N
SMILES: Cc1cnc2cccc(C)c2c1
Mol. weight [g/mol]: 157.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.99		Crippen Method
logp	2.852		Crippen Method
mcvol	132.610	ml/mol	McGowan Method
rinpol	1424.00		NIST Webbook
rinpol	1424.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R257059&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.