6-Isopropylquinoline

Other names: Quinoline, 6-(1-methylethyl)-
Inchi: InChI=1S/C12H13N/c1-9(2)10-5-6-12-11(8-10)4-3-7-13-12/h3-9H,1-2H3
InchiKey: NKCQEIXYLHACJC-UHFFFAOYSA-N
Formula: C12H13N
SMILES: CC(C)c1ccc2ncccc2c1
Mol. weight [g/mol]: 171.24
CAS: 135-79-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.23		Crippen Method
logp	3.358		Crippen Method
mcvol	146.700	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=C135795&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