

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/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/47-520-2/6-Isopropylquinoline.pdf>

Generated by Cheméo on 2024-04-29 12:56:13.545941815 +0000 UTC m=+16684622.466519130.

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