

Benzo[h]quinoline, 2,3,4-trimethyl-

Inchi:	InChI=1S/C16H15N/c1-10-11(2)14-9-8-13-6-4-5-7-15(13)16(14)17-12(10)3/h4-9H,1-3H3
InchiKey:	HFSGFWFRCPJMHY-UHFFFAOYSA-N
Formula:	C16H15N
SMILES:	<chem>Cc1nc2c(ccc3ccccc32)c(C)c1C</chem>
Mol. weight [g/mol]:	221.30
CAS:	63042-66-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.27		Crippen Method
logp	4.313		Crippen Method
mcvol	183.600	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=C63042660&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/74-013-5/Benzo-h-quinoline-2-3-4-trimethyl.pdf>

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