

1H-Indole, 2-(1,1-dimethylethyl)-

Other names:	Indole, 2-tert-butyl- 2-tert-Butylindole
Inchi:	InChI=1S/C12H15N/c1-12(2,3)11-8-9-6-4-5-7-10(9)13-11/h4-8,13H,1-3H3
InchiKey:	WVPGIDWFLXGCLA-UHFFFAOYSA-N
Formula:	C12H15N
SMILES:	CC(C)(C)c1cc2ccccc2[nH]1
Mol. weight [g/mol]:	173.25
CAS:	1805-65-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	2.983		Crippen Method
mcvol	151.000	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1805658&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

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