

3-Methyl-2-phenylindole

Other names:	1H-Indole, 3-methyl-2-phenyl-Indole, 3-methyl-2-phenyl-
Inchi:	InChI=1S/C15H13N/c1-11-13-9-5-6-10-14(13)16-15(11)12-7-3-2-4-8-12/h2-10,16H,1H3
InchiKey:	KYAXCYQVBBQQHB-UHFFFAOYSA-N
Formula:	C15H13N
SMILES:	<chem>Cc1c(-c2ccccc2)[nH]c2ccccc12</chem>
Mol. weight [g/mol]:	207.27
CAS:	10257-92-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.57		Crippen Method
logp	3.661		Crippen Method
mcvol	169.510	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10257928&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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