

1H-Indole, 2,5-dimethyl-

Other names:	Indole, 2,5-dimethyl- 2,5-Dimethylindole 2,5-dimethyl-1H-indole
Inchi:	InChI=1S/C10H11N/c1-7-3-4-10-9(5-7)6-8(2)11-10/h3-6,11H,1-2H3
InchiKey:	ZFLFWZRPMDXJCW-UHFFFAOYSA-N
Formula:	C10H11N
SMILES:	<chem>Cc1ccc2[nH]c(C)cc2c1</chem>
Mol. weight [g/mol]:	145.20
CAS:	1196-79-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.45		Crippen Method
logp	2.303		Crippen Method
mcvol	122.820	ml/mol	McGowan Method
rinsol	256.65		NIST Webbook
rinsol	256.65		NIST Webbook

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=C1196798&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
rinsol:	Non-polar retention indices

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