1H-Indole, 2,3,5-trimethyl-

Other names: Indole, 2,3,5-trimethyl-
2,3,5-Trimethylindole
Inchi: InChI=1S/C11H13N/c1-7-4-5-11-10(6-7)8(2)9(3)12-11/h4-6,12H,1-3H3
InchiKey: HOFNMMIHFZBKPW-UHFFFAOYSA-N
Formula: C11H13N
SMILES: Cc1ccc2[nH]c(C)c(C)c2c1
Mol. weight [g/mol]: 159.23
CAS: 21296-92-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.92		Crippen Method
logp	2.611		Crippen Method
mcvol	136.910	ml/mol	McGowan Method
rinpol	273.61		NIST Webbook
rinpol	272.57		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21296924&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
rinpol: Non-polar retention indices