2,4-Dimethyl-1H-indole

Inchi: InChI=1S/C10H11N/c1-7-4-3-5-10-9(7)6-8(2)11-10/h3-6,11H,1-2H3
InchiKey: YBUMNVFXMLIKDZ-UHFFFAOYSA-N
Formula: C10H11N
SMILES: Cc1cc2c(C)cccc2[nH]1
Mol. weight [g/mol]: 145.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.45		Crippen Method
logp	2.303		Crippen Method
mcvol	122.820	ml/mol	McGowan Method
rinpol	1485.00		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=R586179&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
rinpol: Non-polar retention indices