

6-propoxy-indole

Inchi: InChI=1S/C11H13NO/c1-2-7-13-10-4-3-9-5-6-12-11(9)8-10/h3-6,8,12H,2,7H2,1H3
InchiKey: JDVBDXYRDRFRP-UHFFFAOYSA-N
Formula: C11H13NO
SMILES: CCCOc1ccc2cc[nH]c2c1
Mol. weight [g/mol]: 175.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.45		Crippen Method
logp	2.475		Crippen Method
mcvol	142.780	ml/mol	McGowan Method
rinpol	1726.00		NIST Webbook
rinpol	1732.00		NIST Webbook
rinpol	1726.00		NIST Webbook
ripol	2916.00		NIST Webbook
ripol	2928.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R135256&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices

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