6-isopropoxy-indole

Inchi: InChI=1S/C11H13NO/c1-8(2)13-10-4-3-9-5-6-12-11(9)7-10/h3-8,12H,1-2H3
InchiKey: VYUAYKJMJXXCLP-UHFFFAOYSA-N
Formula: C11H13NO
SMILES: CC(C)Oc1ccc2cc[nH]c2c1
Mol. weight [g/mol]: 175.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.56		Crippen Method
logp	2.473		Crippen Method
mcvol	142.780	ml/mol	McGowan Method
rinpol	1649.00		NIST Webbook
rinpol	1657.00		NIST Webbook
rinpol	1649.00		NIST Webbook
ripol	2800.00		NIST Webbook
ripol	2814.00		NIST Webbook
ripol	2800.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R135221&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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