1H-Indole, 6-methoxy-

Other names: Indole, 6-methoxy-
6-Methoxyindole
6-Methoxy-1H-indole
Inchi: InChI=1S/C9H9NO/c1-11-8-3-2-7-4-5-10-9(7)6-8/h2-6,10H,1H3
InchiKey: QJRWYBIKLXNYLF-UHFFFAOYSA-N
Formula: C9H9NO
SMILES: COc1ccc2cc[nH]c2c1
Mol. weight [g/mol]: 147.17
CAS: 3189-13-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.61		Crippen Method
logp	1.695		Crippen Method
mcvol	114.600	ml/mol	McGowan Method
rinpol	1574.00		NIST Webbook
rinpol	1563.00		NIST Webbook
ripol	2826.00		NIST Webbook
ripol	2807.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3189137&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