

6-Ethoxyindole

Other names:	6-ethoxyindole 6-ethoxy-1H-indole
Inchi:	InChI=1S/C10H11NO/c1-2-12-9-4-3-8-5-6-11-10(8)7-9/h3-7,11H,2H2,1H3
InchiKey:	RPMWEGXHQSEPPH-UHFFFAOYSA-N
Formula:	C10H11NO
SMILES:	CCOc1ccc2cc[nH]c2c1
Mol. weight [g/mol]:	161.20
CAS:	37865-86-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.03		Crippen Method
logp	2.085		Crippen Method
mcpol	128.690	ml/mol	McGowan Method
ripol	1620.00		NIST Webbook
ripol	1638.00		NIST Webbook
ripol	1620.00		NIST Webbook
ripol	1632.00		NIST Webbook
ripol	2842.00		NIST Webbook
ripol	2861.00		NIST Webbook
ripol	2842.00		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=C37865864&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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