

4-Ethyl-2-methoxypyrrole

Inchi: InChI=1S/C7H11NO/c1-3-6-4-7(9-2)8-5-6/h4-5,8H,3H2,1-2H3
InchiKey: HOYOCRLVRNESOA-UHFFFAOYSA-N
Formula: C7H11NO
SMILES: CCc1c[nH]c(OC)c1
Mol. weight [g/mol]: 125.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.61		Crippen Method
logp	1.104		Crippen Method
mcvol	105.880	ml/mol	McGowan Method
ripol	1680.00		NIST Webbook
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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=R633582&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/92-718-3/4-Ethyl-2-methoxypyrrole.pdf>

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