

2-ethyl-3-methylpyrrole

Inchi: InChI=1S/C7H11N/c1-3-8-6-4-5-7(8)2/h4-6H,3H2,1-2H3
InchiKey: WBSWPBIIIRQMFK-UHFFFAOYSA-N
Formula: C7H11N
SMILES: CCn1cccc1C
Mol. weight [g/mol]: 109.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.21		Crippen Method
logp	1.816		Crippen Method
mcvol	100.010	ml/mol	McGowan Method
rinpole	964.00		NIST Webbook
rinpole	964.00		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=R236601&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/38-875-9/2-ethyl-3-methylpyrrole.pdf>

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