

1-methyl-1H-pyrrole-2-acetonitrile

Inchi: InChI=1S/C6H6N2/c1-8-4-2-3-6(8)5-7/h2-4H,1H3
InchiKey: JRQSGIQEBOZPHK-UHFFFAOYSA-N
Formula: C6H6N2
SMILES: Cn1cccc1C#N
Mol. weight [g/mol]: 106.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.11		Crippen Method
logp	0.897		Crippen Method
mcvol	87.300	ml/mol	McGowan Method
rinpol	1118.00		NIST Webbook
ripol	1598.00		NIST Webbook
ripol	1598.00		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=R299880&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

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