

Pyrrole-2-carbonitrile

Inchi: InChI=1S/C5H4N2/c6-4-5-2-1-3-7-5/h1-3,7H
InchiKey: BQMPGKPTOHKYHS-UHFFFAOYSA-N
Formula: C5H4N2
SMILES: N#Cc1ccc[nH]1
Mol. weight [g/mol]: 92.10
CAS: 4513-94-4

Physical Properties

Property code	Value	Unit	Source
ie	8.70	eV	NIST Webbook
ie	9.08	eV	NIST Webbook
log10ws	-1.04		Crippen Method
logp	0.404		Crippen Method
mcvol	73.210	ml/mol	McGowan Method

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=C4513944&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/108-258-6/Pyrrole-2-carbonitrile.pdf>

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