

Methyl pyrrole-2-carboxylate

Other names: 1H-Pyrrole-2-carboxylic acid,methyl ester
Inchi: InChI=1S/C6H7NO2/c1-9-6(8)5-3-2-4-7-5/h2-4,7H,1H3
InchiKey: VONGYFFEWFJHNP-UHFFFAOYSA-N
Formula: C6H7NO2
SMILES: COC(=O)c1ccc[nH]1
Mol. weight [g/mol]: 125.13
CAS: 1193-62-0

Physical Properties

Property code	Value	Unit	Source
ie	8.65 ± 0.05	eV	NIST Webbook
log10ws	-0.93		Crippen Method
logp	0.319		Crippen Method
mcvol	93.360	ml/mol	McGowan Method
ripol	2058.00		NIST Webbook
ripol	2058.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1193620&Units=SI>
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>

Legend

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

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