

Methyl nicotinate

Other names:	3-(Carbomethoxy)pyridine 3-(Methoxycarbonyl)pyridine 3-Pyridinecarboxylic acid, methyl ester Methyl 3-pyridinecarboxylate Methyl ester of pyridine-3-carboxylic acid NSC 13126 Nicometh Nicotinic acid, methyl ester Nikomet m-(Methoxycarbonyl)pyridine
Inchi:	InChI=1S/C7H7NO2/c1-10-7(9)6-3-2-4-8-5-6/h2-5H,1H3
InchiKey:	YNBADRVTZLEFNH-UHFFFAOYSA-N
Formula:	C7H7NO2
SMILES:	COC(=O)c1cccnc1
Mol. weight [g/mol]:	137.14
CAS:	93-60-7

Physical Properties

Property code	Value	Unit	Source
affp	925.60	kJ/mol	NIST Webbook
basg	893.80	kJ/mol	NIST Webbook
hvap	61.20 ± 0.20	kJ/mol	NIST Webbook
ie	9.90 ± 0.10	eV	NIST Webbook
ie	9.25	eV	NIST Webbook
log10ws	-0.46		Aqueous Solubility Prediction Method
log10ws	-0.46		Estimated Solubility Method
logp	0.868		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
rinpol	1145.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1141.20		NIST Webbook
rinpol	1140.10		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1136.60		NIST Webbook

rinpol	1098.00		NIST Webbook
rinpol	1139.20		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1137.40		NIST Webbook
rinpol	1137.40		NIST Webbook
rinpol	1152.20		NIST Webbook
rinpol	1149.00		NIST Webbook
ripol	1739.00		NIST Webbook
ripol	1779.00		NIST Webbook
ripol	1743.00		NIST Webbook
ripol	1739.00		NIST Webbook
ripol	1779.00		NIST Webbook
ripol	1793.00		NIST Webbook
ripol	1779.00		NIST Webbook
tb	482.20	K	NIST Webbook
tb	477.20	K	NIST Webbook
tf	315.40	K	Aqueous Solubility Prediction Method

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Aqueous Solubility Prediction Method:

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

Estimated Solubility Method:

http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C93607&Units=SI>

Legend

affp:	Proton affinity
basg:	Gas basicity
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point

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