

4-Pyridinecarboxylic acid, methyl ester

Other names:	Isonicotinic acid, methyl ester Methyl isonicotinate Methyl 4-pyridinecarboxylate 4-Methoxycarbonylpyridine 4-Carbomethoxypyridine Pyridine-4-carboxylic acid, methyl ester
Inchi:	InChI=1S/C7H7NO2/c1-10-7(9)6-2-4-8-5-3-6/h2-5H,1H3
InchiKey:	OLXYLDUSSBULGU-UHFFFAOYSA-N
Formula:	C7H7NO2
SMILES:	<chem>COC(=O)c1ccncc1</chem>
Mol. weight [g/mol]:	137.14
CAS:	2459-09-8

Physical Properties

Property code	Value	Unit	Source
affp	926.60	kJ/mol	NIST Webbook
basg	894.70	kJ/mol	NIST Webbook
hvap	59.40 ± 0.10	kJ/mol	NIST Webbook
hvap	65.40 ± 1.40	kJ/mol	NIST Webbook
log10ws	-1.48		Crippen Method
logp	0.868		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
rinpol	1125.00		NIST Webbook
ripol	1763.00		NIST Webbook
ripol	1782.00		NIST Webbook
ripol	1782.00		NIST Webbook
ripol	1804.00		NIST Webbook
tb	481.20	K	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2459098&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
hvap:	Enthalpy of vaporization at standard conditions
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
tb:	Normal Boiling Point Temperature

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