

Ethyl nicotinate

Other names:	3-Pyridinecarboxylic acid, ethyl ester
	Nicotinic acid, ethyl ester
	«beta»-Pyridinecarboxylic acid ethyl ester
	Ba 2673
	Ethyl 3-pyridinecarboxylate
	Ignicut
	Ignocut
	Mucotherm
	Nicaethan
	Nikethan
	Nikithan
	3-(Ethoxycarbonyl)pyridine
	3-Carbethoxypyridine
	NSC 8872
Inchi:	InChI=1S/C8H9NO2/c1-2-11-8(10)7-4-3-5-9-6-7/h3-6H,2H2,1H3
InchiKey:	XBLVHTDFJBKJLG-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	CCOC(=O)c1cccnc1
Mol. weight [g/mol]:	151.16
CAS:	614-18-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.90		Crippen Method
logp	1.258		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
rinpol	1218.00		NIST Webbook
rinpol	1196.00		NIST Webbook
rinpol	1191.00		NIST Webbook
rinpol	1218.00		NIST Webbook
rinpol	1224.00		NIST Webbook
rinpol	1183.00		NIST Webbook
rinpol	1191.00		NIST Webbook
rinpol	1190.00		NIST Webbook
ripol	1771.00		NIST Webbook
ripol	1782.00		NIST Webbook
tb	497.20	K	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C614186&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
tb:	Normal Boiling Point Temperature

Latest version available from:

<https://www.chemeo.com/cid/63-622-1/Ethyl-nicotinate.pdf>

Generated by Cheméo on 2025-12-06 02:50:41.912286248 +0000 UTC m=+4737639.442326903.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.