

4-Pyridinecarboxylic acid, ethyl ester

Other names:	Isonicotinic acid, ethyl ester «gamma»-Pyridinecarboxylic acid ethyl ester Ethyl isonicotinate Ethyl 4-pyridinecarboxylate 4-Carbethoxypyridine 4-Carboethoxypyridine
Inchi:	InChI=1S/C8H9NO2/c1-2-11-8(10)7-3-5-9-6-4-7/h3-6H,2H2,1H3
InchiKey:	MCRPKBUFXAKDKI-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	CCOC(=O)c1ccncc1
Mol. weight [g/mol]:	151.16
CAS:	1570-45-2

Physical Properties

Property code	Value	Unit	Source
ie	9.80 ± 0.10	eV	NIST Webbook
log10ws	-1.90		Crippen Method
logp	1.258		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
rinpol	1201.00		NIST Webbook
ripol	1755.00		NIST Webbook
tb	492.70	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	365.20	K	1.00	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=C1570452&Units=SI>

Legend

ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure

Latest version available from:

<https://www.chemeo.com/cid/22-103-2/4-Pyridinecarboxylic-acid-ethyl-ester.pdf>

Generated by Cheméo on 2025-12-05 19:37:16.17929928 +0000 UTC m=+4711633.709339949.

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