

Nicametate

Other names:

3-Pyridinecarboxylic acid, 2-(diethylamino)ethyl ester
Nicotinic acid, 2-(diethylamino)ethyl ester
2-(Diethylamino)ethyl nicotinate
Eucast

Inchi:

InChI=1S/C12H18N2O2/c1-3-14(4-2)8-9-16-12(15)11-6-5-7-13-10-11/h5-7,10H,3-4,8-9H

InchiKey:

JVWOCHRRRAWHKLT-UHFFFAOYSA-N

Formula:

C12H18N2O2

SMILES:

CCN(CC)CCOC(=O)c1cccnc1

Mol. weight [g/mol]:

222.28

CAS:

3099-52-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.14		Crippen Method
logp	1.580		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
rinpol	1648.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1648.00		NIST Webbook
rinpol	1608.00		NIST Webbook

Sources

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>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C3099523&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

Latest version available from:

<https://www.cheméo.com/cid/39-260-0/Nicametate.pdf>

Generated by Cheméo on 2024-04-28 03:47:29.316210513 +0000 UTC m=+16565298.236787826.

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