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: JVWOCHRRAWHKLT-UHFFFAOYSA-N
Formula: C12H18N2O2
SMILES: CCN(CC)CCOC(=O)c1cccnc1
Mol. weight [g/mol]: 222.29

Physical Properties

Property code	Value	Unit	Source
af	0.6452		Cheméo Relay (1.0)
hf	-277.03	kJ/mol	Cheméo Relay (1.0)
hvap	75.82	kJ/mol	Cheméo Relay (1.0)
ie	8.80	eV	Cheméo Relay (1.0)
log10ws	-1.15		Cheméo Relay (1.0)
logp	1.580		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	2300.59	kPa	Cheméo Relay (1.0, beta)
rinpol	1648.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1648.00		NIST Webbook
tb	572.96	K	Cheméo Relay (1.0)
tc	771.20	K	Cheméo Relay (1.0)
tf	278.27	K	Cheméo Relay (1.0)
vc	0.661	m3/kmol	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3099523&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume