3-Pyridinecarboxamide, N,N-diethyl-

Other names:

3-Pyridinecarboxamide, N,N-diethyl-
Nicotinamide, N,N-diethyl-
Anacardone
Anacordone
Astrocar
Canfodiamina
Carbamidal
Cardamine
Cardiamid
Cardiamide
Cardiamine
Cardimon
Coracon
Coramine
Cordiamin
Cordiamine
Corediol
Cormed
Cormid
Cormotyl
Cornotone
Corvin
Corvitol
Corvotone
Diethylnicotinamide
Dynacoryl
Eucoran
Kordiamin
N,N-Diethylnicotinamide
Ni-Cor
Niamine
Nicamide
Nicetamide
Nicethamide
Nicorine
Nicotinic acid diethylamide
Nikardin
Niketamide
Niketharol
Nikethyl

Nikorin
Percoral
Pyricardyl
Pyridine-3-carboxydiethylamide
Pyridine-3-carboxylic acid diethylamide
Reformin
Rehormin
Salvacard
Sancora
Solyacord
Stimulin
Ventramine
«beta»-Pyrimidum
Camphozone
Cardiagen
Cardiamina
Citocor
Coraetamidum
Coraethamide
Coraethamidum
Coralept
Coravita
Corazone
Cordiamid
Corditon
Cordynil
Corespin
Corethamide
Coretone
Corivo
Corotonin
Corovit
Corvitan
Corywas
Danamine
Diaethyl-nicotinamid
Diethyl-Nicotamide
Dietilamide-Carbopiridina
Dinacoryl
Dynamicarde
Elitone
Hansacor
Inicardio

	Kardiamid
	Kardonyl
	Leptamin
	Mediamid
	Nicordamin
	Nicoryl
	Niketamid
	Niketilamid
	Nikotin
	Niquetamida
	Procardine
	Procorman
	Salvacorin
	Stellamine
	Stiminol
	Tonocard
	Tonocor
	Vasazol
	Diethylamid kyseliny nikotinove
	N,N-Diethyl-3-pyridinecarboxamide
	Nisetamide
	Coractiv N
	Ecoran
	Niketamine
	3-(N,N-Diethylcarbamoyl)pyridine
Inchi:	InChI=1S/C10H14N2O/c1-3-12(4-2)10(13)9-6-5-7-11-8-9/h5-8H,3-4H2,1-2H3
InchiKey:	NCYVXEGFNDZQCU-UHFFFAOYSA-N
Formula:	C10H14N2O
SMILES:	CCN(CC)C(=O)c1cccnc1
Mol. weight [g/mol]:	178.24

Physical Properties

Property code	Value	Unit	Source
af	0.5298		Cheméo Relay (1.0)
affp	940.90	kJ/mol	NIST Webbook
basg	909.00	kJ/mol	NIST Webbook
hf	-100.61	kJ/mol	Cheméo Relay (1.0)
hvap	67.88	kJ/mol	Cheméo Relay (1.0)
ie	8.65	eV	NIST Webbook

log10ws	-1.05		Cheméo Relay (1.0)
logp	1.564		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2728.59	kPa	Cheméo Relay (1.0, beta)
rinpol	1515.00		NIST Webbook
rinpol	1494.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1464.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1487.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1511.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1466.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1506.00		NIST Webbook
ripol	2319.00		NIST Webbook
ripol	2319.00		NIST Webbook
ripol	2319.00		NIST Webbook
ripol	2375.00		NIST Webbook
ripol	2386.00		NIST Webbook
ripol	2399.00		NIST Webbook
ripol	2353.00		NIST Webbook

ripol	2375.00		NIST Webbook
ripol	2353.00		NIST Webbook
tb	571.20	K	NIST Webbook
tc	774.01	K	Cheméo Relay (1.0)
tf	314.08	K	Cheméo Relay (1.0)

Sources

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):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C59267&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor
affp: Proton affinity
basg: Gas basicity
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point