

nalidixic acid

Other names:

1,4-Dihydro-1-ethyl-7-methyl-4-oxo-1,8-naphthyridine-3-carboxylic acid
1,8-Naphthyridine-3-carboxylic acid, 1-ethyl-1,4-dihydro-7-methyl-4-oxo-
1-Aethyl-7-methyl-1,8-naphthyridin-4-on-3-karbonsaeure
1-Ethyl-1,4-dihydro-7-methyl-4-oxo-1,8-naphthyridine-3-carboxylic acid
1-Ethyl-1,4-dihydro-7-methyl-4-oxo-1,8-naphthyridine-3-carboxylic acid
1-Ethyl-1,4-dihydro-7-methyl-4-oxo-1,8-naphthyridine-3-carboxylic acid (nalidixic acid)
1-Ethyl-7-methyl-1,4-dihydro-1,8-naphthyridin-4-one-3-carboxylic acid
1-ethyl-7-methyl-4-oxo-1,4-dihydro-1,8-naphthyridine-3-carboxylic acid
3-Carboxy-1-ethyl-7-methyl-1,8-naphthidin-4-one
3-Carboxy-1-ethyl-7-methyl-1,8-naphthyridin-4-one
Acide 1-etil-7-metil-1,8-naftiridin-4-one-3-carbossilico
Acide nalidixico
Acide nalidixique
Betaxina
Cybis
Dixiben
Dixinal
Eucisten
Eucistin
Innoxalomn
Innoxalon
Jicsron
Kusnarin
NCI-C56199
NSC-82174
Nacid
Nalidic acid
Nalidicron
Nalidixan
Nalidixane
Nalidixate
Nalidixin
Nalidixinic acid
Nalitucsan
Nalix
Nalurin
Narigix
Naxuril
NegGram
Negram

Nevigramon

Nicelate

Nogram

Poleon

Sicmylon

Specifen

Specifin

Unaserus

Uralgin

Uriben

Uriclar

Urisal

Urodixin

Uroman

Uroneg

Uronidix

Uropan

WIN 18,320

WIN 18320

Wintomylon

Inchi:

InChI=1S/C12H12N2O3/c1-3-14-6-9(12(16)17)10(15)8-5-4-7(2)13-11(8)14/h4-6H,3H2,1-

InchiKey:

MHWLWQUZZRMNGJ-UHFFFAOYSA-N

Formula:

C12H12N2O3

SMILES:

CCn1cc(C(=O)O)c(=O)c2ccc(C)nc21

Mol. weight [g/mol]:

232.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.66		Aqueous Solubility Prediction Method
logp	1.423		Crippen Method
mcvol	169.990	ml/mol	McGowan Method
tf	500.90	K	Thermodynamic properties of Nalidixic and Oxolinic acids: Experimental and computational study
tf	502.55	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	35.92	kJ/mol	501.90	NIST Webbook
hfust	35.92	kJ/mol	501.90	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Thermodynamic properties of Nalidixic and Oxolinic acids: Experimental and Computational Study

<https://www.doi.org/10.1016/j.tca.2019.178411>

Composition Prediction Method:

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C389082&Units=SI>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

hfust: Enthalpy of fusion at a given temperature

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

tf: Normal melting (fusion) point

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