Oxolinic acid

Other names:	1,3-Dioxolo[4,5-g]quinoline-7-carboxylic acid, 5-ethyl-5,8-dihydro-8-oxo-
	1-Ethyl-1,4-dihydro-6,7-methylenedioxy-4-oxo-3-quinoline-carboxylic acid (oxolinic acid)
	1-Ethyl-1,4-dihydro-6,7-methylenedioxy-4-oxo-3-quinolinecarboxylic acid
	1-Ethyl-6,7-methylenedioxy-4-quinolone-3-carboxylic acid
	5-Ethyl-5,8-dihydro-8-oxo-1,3-dioxolo(4,5-g)quinoline-7-carboxylic acid
	5-ethyl-5,8-dihydro-8-oxo-1,3-dioxolo[4,5-g]quinoline-7-carboxylic acid
	5-ethyl-8-oxo-5,8-dihydro-[1,3]dioxolo[4,5-g]quinoline-7-carboxylic acid
	Dioxacin
	Emyrenil
	Gramurin
	Inoxyl
	NSC-110364
	Nidantin
	Oksaren
	Ossian
	Oxoboi
	Oxolinic
	Pietil
	Prodoxal
	Prodoxol
	Starner
	Ultibid
	Urinox
	Uritrate
	Uro-alvar
	Urotrate
	Uroxin
	Uroxol
	Utibid
	W 4565
Inchi:	InChI=1S/C13H11NO5/c1-2-14-5-8(13(16)17)12(15)7-3-10-11(4-9(7)14)19-6-18-10/h3-5H
InchiKey:	KYGZCKSPAKDVKC-UHFFFAOYSA-N
Formula:	C13H11NO5
SMILES:	CCn1cc(C(=O)O)c(=O)c2cc3c(cc21)OCO3
Mol. weight [g/mol]:	261.23
CAS:	14698-29-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.59		Aqueous Solubility Prediction Method
logp	1.448		Crippen Method
mcvol	174.980	ml/mol	McGowan Method
tf	592.20	K	Thermodynamic properties of Nalidixic and Oxolinic acids: Experimental and computational study

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	43.59	kJ/mol	592.50	NIST Webbook

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14698294&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermodynamic properties of Nalidixic and Oxolinic acids: Experimental and computational study:	https://www.doi.org/10.1016/j.tca.2019.178411

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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