Niflumic acid

Other names:	2-(3-(Trifluoromethyl)-phenyl)aminonicotinic acid
	2-[3-(Trifluoromethyl)anilino]-3-pyridinecarboxylic acid
	2-[3-(Trifluoromethyl)anilino]nicotinic acid
	2-[3-(Trifluoromethyl)anilino]nicotinic acid (niflumic acid)
	2-[[3-(trifluoromethyl)phenyl]amino]-3-pyridinecarboxylic acid
	3- pyridinecarboxylic acid, 2-[[3-(trifluoromethyl)phenyl]amino]-
	3-Pyridinecarboxylic acid, 2-[[3-(trifluoromethyl)phenyl]amino]-
	Acide niflumique
	Acido niflumico
	Actol
	Actol, analgesic
	Flogovital
	Forenol
	Landruma
	Nicotinic acid, 2-(«alpha»,«alpha»,«alpha»-trifluoro-m-toluidino)-
	Nicotinic acid, 2-(Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluoro-m-toluidino)-
	Niflamol
	Nifluminic acid
	Nifluril
	UP 83
Inchi:	InChI=1S/C13H9F3N2O2/c14-13(15,16)8-3-1-4-9(7-8)18-11-10(12(19)20)5-2-6-17-11/h1
InchiKey:	JZFPYUNJRRFVQU-UHFFFAOYSA-N
Formula:	C13H9F3N2O2
SMILES:	O=C(O)c1cccnc1Nc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	282.22
CAS:	4394-00-7

Physical Properties

Property code	Value	Unit	Source
hsub	130.20 ± 0.80	kJ/mol	NIST Webbook
hvap	107.50	kJ/mol	NIST Webbook
log10ws	-4.00		Aqueous Solubility Prediction Method
logp	3.542		Crippen Method
mcvol	179.220	ml/mol	McGowan Method
rinpol	2093.00		NIST Webbook

tf	477.15	K	Determination, correlation and prediction of the solubilities of niflumic acid, clofenamic acid and tolfenamic acid in supercritical CO2
tf	476.00 ± 0.10	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	36.50	kJ/mol	478.00	NIST Webbook
hfust	35.70	kJ/mol	476.40	NIST Webbook
hfust	32.73	kJ/mol	477.20	NIST Webbook
hfust	38.00	kJ/mol	476.00	NIST Webbook
hsubt	127.80 ± 0.80	kJ/mol	375.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4394007&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Determination, correlation and prediction of the solubilities of niflumic acid, clofenamic acid and tolfenamic acid in supercritical CO2:	https://www.doi.org/10.1016/j.fluid.2015.02.007
Solubilities of Organic Semiconductors and Nonsteroidal Anti-inflammatory Drugs in Pure and Mixed Organic Solvents: Measurement and Modeling:	https://www.doi.org/10.1021/acs.jced.8b00536
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: **With Hansen Solubility Parameter:**	http://link.springer.com/article/10.1007/BF02311772

Legend

hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point