Flufenamic acid

Other names:

2-((3-(Trifluoromethyl)phenyl)amino)benzoic acid
2-((3-Triflуromethyl)phenyl)aminobenzoic acid
2-[[3-(Trifluoromethyl)phenyl]amino]benzoic acid (flufenamic acid)
3'-Trifluoromethyldiphenylamine-2-carboxylic acid
ANT-1
Achless
Acido flufenamico
Ansatin
Anthranilic acid, N-(«alpha»,«alpha»,«alpha»-trifluoro-m-tolyl)-
Arlef
Benzoic acid, 2-[[3-(trifluoromethyl)phenyl]amino]-
C.I. 440
CI 440
CN-27,554
CN-27544
Flufacid
Flufenaminsaeure
Fluore-200
Fluphenamic acid
Fullsafe
INF 1837
Lanceat
Meralen
N-((m-Trifluoromethyl)phenyl)-2-aminobenzoic acid
N-(3-Trifluoromethylphenyl)-anthranilic acid
N-(«alpha»,«alpha»,«alpha»-Trifluoro-m-tolyl)anthranilic acid
NSC 219007
NSC-82699
Nichisedan
Paraflu
Parlef
Parlif
Plostene
Reumajust A
Ristogen
Sastridex
Surika
TVX 916
Tecramine

Inchi:

InChI=1S/C14H10F3NO2/c15-14(16,17)9-4-3-5-10(8-9)18-12-7-2-1-6-11(12)13(19)20/h1

InchiKey: LPEPZBJOKDYZAD-UHFFFAOYSA-N
Formula: C14H10F3NO2
SMILES: O=C(O)c1ccccc1Nc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 281.23
CAS: 530-78-9

Physical Properties

Property code	Value	Unit	Source
gf	-485.38	kJ/mol	Joback Method
hf	-690.59	kJ/mol	Joback Method
hfus	31.93	kJ/mol	Joback Method
hsub	121.20 ± 0.70	kJ/mol	NIST Webbook
hvap	101.60	kJ/mol	NIST Webbook
log10ws	-3.59		Aqueous Solubility Prediction Method
log10ws	-4.62		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	4.147		Crippen Method
mcvol	183.330	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
rinpol	1990.00		NIST Webbook
rinpol	1932.00		NIST Webbook
rinpol	1932.00		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	1950.00		NIST Webbook
tb	773.84	K	Joback Method
tc	985.67	K	Joback Method
tf	404.65	K	Aqueous Solubility Prediction Method
vc	0.707	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.64	J/mol×K	879.76	Joback Method
cpg	549.41	J/mol×K	915.06	Joback Method

cpg	556.56	J/mol×K	950.37	Joback Method
cpg	514.04	J/mol×K	773.84	Joback Method
cpg	524.03	J/mol×K	809.15	Joback Method
cpg	533.21	J/mol×K	844.45	Joback Method
cpg	563.18	J/mol×K	985.67	Joback Method
hfust	26.70	kJ/mol	405.00	NIST Webbook
hfust	27.00	kJ/mol	407.30	NIST Webbook
hsubt	119.40 ± 0.70	kJ/mol	357.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C530789&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume