

Mefenamic Acid

Other names:	2-((2,3-Dimethylphenyl)amino)benzoic acid
	2-Diphenylaminecarboxylic acid, 2',3'-dimethyl-
	2-[(2,3-Dimethylphenyl)amino]benzoic acid (mefenamic acid)
	AGN-1255
	Acide mefenamique
	Anthranilic acid, N-2,3-xylyl-
	Bafameritin-M
	Bafhameritin-M
	Benzoic acid, 2-[(2,3-dimethylphenyl)amino]-
	Bonabol
	CL 473
	CN-35355
	Coslan
	HL 1
	INF 3355
	In-M
	Lysalgo
	Mefacit
	Mefanamic acid
	Mefenacid
	Mefenaminsaeure
	Mephenamic acid
	Mephenaminic acid
	Methenamic acid
	N-(2,3-Dimethylphenyl)anthranilic acid
	N-(2,3-Xylyl)-2-aminobenzoic acid
	N-(2,3-Xylyl)anthranilic acid
	NSC 94437
	Namphen
	Parkemed
	Ponalar
	Ponstan
	Ponstan forte
	Ponstel
	Ponstil
	Ponstyl
	Pontal
	Tamany Bonsan
	Tanston
	Vialidon

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

CAS:

InChI=1S/C15H15NO2/c1-10-6-5-9-13(11(10)2)16-14-8-4-3-7-12(14)15(17)18/h3-9,16H,

HYJBABOKPJLUIN-UHFFFAOYSA-N

C15H15NO2

Cc1cccc(Nc2ccccc2C(=O)O)c1C

241.29

61-68-7

Physical Properties

Property code	Value	Unit	Source
gf	95.00	kJ/mol	Joback Method
hf	-125.62	kJ/mol	Joback Method
hfus	32.31	kJ/mol	Joback Method
hsub	136.30 ± 0.80	kJ/mol	NIST Webbook
hvap	85.38	kJ/mol	Joback Method
log10ws	-3.38		Aqueous Solubility Prediction Method
logp	3.745		Crippen Method
mcvol	192.110	ml/mol	McGowan Method
pc	2850.52	kPa	Joback Method
rinpol	2201.00		NIST Webbook
rinpol	2201.00		NIST Webbook
tb	807.12	K	Joback Method
tc	1030.77	K	Joback Method
tf	503.10	K	Solubility and pKa of select pharmaceuticals in water, ethanol, and 1-octanol
tf	503.65	K	Aqueous Solubility Prediction Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.21	J/mol×K	993.50	Joback Method
cpg	540.37	J/mol×K	807.12	Joback Method
cpg	552.03	J/mol×K	844.40	Joback Method
cpg	562.80	J/mol×K	881.67	Joback Method
cpg	572.72	J/mol×K	918.95	Joback Method

cpg	581.84	J/mol×K	956.22	Joback Method
cpg	597.89	J/mol×K	1030.77	Joback Method
hfust	38.70	kJ/mol	503.50	NIST Webbook
hfust	38.25	kJ/mol	503.60	NIST Webbook
hfust	38.20	kJ/mol	503.60	NIST Webbook
hsubt	132.70 ± 0.80	kJ/mol	377.50	NIST Webbook

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
Measurement and modeling of mefenamic acid solubility in supercritical carbon dioxide:	https://www.doi.org/10.1016/j.fluid.2011.09.031
Solubility and Partition Coefficients of pharmaceuticals in water, ethanol, and toluene:	https://www.doi.org/10.1016/j.jct.2010.07.001
Thermodynamic Data of Mefenamic Acid Crystals in Different Classes of Organic Solvents:	https://www.doi.org/10.1021/je400714f
Joback Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61687&Units=SI
Thermodynamic Study of Solubility for Imatinib Mesylate in Nine McGowan's Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan's Method:	https://www.doi.org/10.1021/acs.jced.8b00551
Crippen Method:	http://link.springer.com/article/10.1007/BF02311772
	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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