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: 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,
InchiKey: HYYBABOKPJLUIN-UHFFFAOYSA-N
Formula: C15H15NO2
SMILES: Cc1cccc(Nc2ccccc2C(=O)O)c1C
Mol. weight [g/mol]: 241.29
CAS: 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	503.65	K	Aqueous Solubility Prediction Method
tf	503.10	K	Solubility and pKa of select pharmaceuticals in water, ethanol, and 1-octanol
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	590.21	J/mol×K	993.50	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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61687&Units=SI
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermodynamic Study of Solubility for Imatinib Mesylate in Nine Monosolvents and Two Binary Solvent Mixtures from 278.15 to 318.15 K:	https://www.doi.org/10.1021/acs.jced.8b00551
Measurement and modeling of mefenamic acid solubility in supercritical carbon dioxide:	https://www.doi.org/10.1016/j.fluid.2011.09.031
Joback Method	https://en.wikipedia.org/wiki/Joback_method
Solubility and pKa of select pharmaceuticals in water, ethanol, and 1-octanol:	https://www.doi.org/10.1016/j.jct.2010.07.001
Solubility and Dissolution Thermodynamic Data of Mefenamic Acid Crystals in Different Classes of Organic Solvents:	https://www.doi.org/10.1021/je400714f

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