Mesalamine

Other names:	2-Hydroxy-5-aminobenzoic acid
	5-ASA
	5-Amino-2-hydroxybenzoic acid
	5-Aminosalicylic acid
	Asacol
	Asacolitin
	Benzoic acid, 5-amino-2-hydroxy-
	Canasa
	Claversal
	Fisalamine
	Lialda
	Lixacol
	Mesalazine
	Mesasal
	NSC 38877
	Pentasa
	Rowasa
	Salicylic acid, 5-amino-
	Salofalk
	m-Aminosalicylic acid
	p-Aminosalicylsaeure
Inchi:	InChI=1S/C7H7NO3/c8-4-1-2-6(9)5(3-4)7(10)11/h1-3,9H,8H2,(H,10,11)
InchiKey:	KBOPZPXVLCULAV-UHFFFAOYSA-N
Formula:	C7H7NO3
SMILES:	Nc1ccc(O)c(C(=O)O)c1
Mol. weight [g/mol]:	153.14
CAS:	89-57-6

Physical Properties

Property code	Value	Unit	Source
gf	-243.07	kJ/mol	Joback Method
hf	-371.08	kJ/mol	Joback Method
hfus	24.21	kJ/mol	Joback Method
hvap	81.19	kJ/mol	Joback Method
log10ws	-2.26		Aqueous and cosolvent solubility data for drug-like organic compounds

log10ws	-2.18		Aqueous Solubility Prediction Method
logp	0.673		Crippen Method
mcvol	109.020	ml/mol	McGowan Method
pc	6796.39	kPa	Joback Method
tb	690.42	K	Joback Method
tc	918.13	K	Joback Method
tf	556.65	K	Aqueous Solubility Prediction Method
tf	554.15	K	Solubility of 5-Amino Salicylic Acid in Different Solvents at Various Temperatures
vc	0.340	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.08	J/mol×K	880.18	Joback Method
cpg	277.00	J/mol×K	690.42	Joback Method
cpg	283.98	J/mol×K	728.37	Joback Method
cpg	290.51	J/mol×K	766.32	Joback Method
cpg	296.65	J/mol×K	804.27	Joback Method
cpg	302.48	J/mol×K	842.23	Joback Method
cpg	313.51	J/mol×K	918.13	Joback Method
hfust	67.20	kJ/mol	543.20	NIST Webbook

Sources

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C89576&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Solubility of 5-Amino Salicylic Acid in Different Solvents at Various Temperatures: https://www.doi.org/10.1021/je900646u

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume