Pyrazinamide

Other names:	2-Carbamylpyrazine
	2-Pyrazinecarboxamide
	Aldinamid
	Aldinamide
	D-50
	Eprazin
	Farmizina
	MK 56
	NCI-C01785
	NSC 14911
	Novamid
	PZA
	Pirazimida
	Pirazinamid
	Pyrafat
	Pyrazine Carboxylamide
	Pyrazineamide
	Pyrazinecarboxamide
	Pyrazinecarboxylic acid amide
	Pyrazinoic acid amide
	T 165
	Tebrazid
	Unipyranamide
	Zinamide
Inchi:	InChI=1S/C5H5N3O/c6-5(9)4-3-7-1-2-8-4/h1-3H,(H2,6,9)
InchiKey:	IPEHBUMCGVEMRF-UHFFFAOYSA-N
Formula:	C5H5N3O
SMILES:	NC(=O)c1cnccn1
Mol. weight [g/mol]:	123.11
CAS:	98-96-4

Physical Properties

Property code	Value	Unit	Source

hfus	28.14	kJ/mol	Solubility Advantage of Pyrazine-2-carboxamide: Application of Alternative Solvents on the Way to the Future Pharmaceutical Development
hfus	27.10	kJ/mol	Solution thermodynamics of pyrazinamide, isoniazid, and p-aminobenzoic acid in buffers and octanol
log10ws	-0.67		Estimated Solubility Method
log10ws	-0.70		Aqueous Solubility Prediction Method
logp	-0.425		Crippen Method
mcvol	89.060	ml/mol	McGowan Method
rinpol	1250.00		NIST Webbook
ripol	1755.00		NIST Webbook
ripol	1740.00		NIST Webbook
ripol	1755.00		NIST Webbook
tf	461.42	K	Ammonium ionic liquids as green solvents for drugs
tf	462.11	K	Solubility measurements and thermodynamic modeling of pyrazinamide in five different solvent-antisolvent mixtures
tf	461.42	K	Solubility Data as a Response for a Challenge for Formulation Chemists: Imidazolium-Based Ionic Liquids and Antitubercular Antibiotic Medicines
tf	463.00 ± 1.00	K	NIST Webbook
tf	463.55	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	30.28	kJ/mol	463.00	NIST Webbook
hsubt	87.90	kJ/mol	368.00	NIST Webbook

Sources

Ammonium ionic liquids as green solvents for drugs:	https://www.doi.org/10.1016/j.fluid.2012.11.029
Solution thermodynamics of pyrazinamide, isoniazid, and p-aminobenzoic acid in buffers and octanol:	https://www.doi.org/10.1016/j.jct.2015.08.022
Solubilities of pharmaceutical and bioactive compounds in trihexyl(tetradecyl)phosphonium chloride ionic liquid:	https://www.doi.org/10.1016/j.fluid.2015.03.053
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Solubility measurements and thermodynamic modeling of pyrazinamide in five different solvent mixtures:	https://www.doi.org/10.1016/j.fluid.2019.06.004
Solubility Advantage of Pyrazine-2-carboxamide: Application of Alternative Solvents on the Way to the Greener Pharmaceutical Development:	https://www.doi.org/10.1021/je300044x
Thermodynamic study of solubility for pyrazinamide in ten solvents from T= (283.15 to 323.15) K:	https://www.doi.org/10.1016/j.jct.2017.04.014
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98964&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility Data as a Response for a Challenge for Formulation Chemists:	https://www.doi.org/10.1021/acs.jced.6b00201
Solubility studies on the system of trihexyl(tetradecyl)phosphonium bis[(trifluoromethyl)sulfonyl]amide) ionic liquid and pharmaceutical and bioactive compounds:	https://www.doi.org/10.1016/j.fluid.2014.10.033
Imidazolium Based Ionic Liquids and Antibacterial Antibiotic Medicines: Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

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