Pyrazinoic acid

Other names:	1,4-diazinecarboxylic acid
	2-carboxypyrazine
	2-pyrazinecarboxylic acid
	2-pyrazinoic acid
	NSC 13146
	Paradiazinecarboxylic acid
	Piazinecarboxylic acid
	Pyrazine-2-carboxylic acid
	Pyrazinemonocarboxylic acid
	Pyrazoic acid
	pyrazinecarboxylic acid
	pyrazinic acid
Inchi:	InChI=1S/C5H4N2O2/c8-5(9)4-3-6-1-2-7-4/h1-3H,(H,8,9)
InchiKey:	NIPZZXUFJPQHNH-UHFFFAOYSA-N
Formula:	C5H4N2O2
SMILES:	O=C(O)c1cnccn1
Mol. weight [g/mol]:	124.10
CAS:	98-97-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.06		Crippen Method
logp	0.175		Crippen Method
mcvol	84.950	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98975&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Low-temperature Heat Capacity and the Standard Molar Enthalpy of Formation of Compound Chromium(III) Tri(2-Pyrazinecarboxylate):	https://www.doi.org/10.1016/j.tca.2012.05.023
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume