2-Methylpyrazine-5-carboxylic acid

Other names:	2-Methyl-5-pyrazine carboxylic acid
	2-Pyrazinecarboxylic acid, 5-methyl-
	5-methylpyrazine-2-carboxylic acid
Inchi:	InChI=1S/C6H6N2O2/c1-4-2-8-5(3-7-4)6(9)10/h2-3H,1H3,(H,9,10)
InchiKey:	RBYJWCRKFLGNDB-UHFFFAOYSA-N
Formula:	C6H6N2O2
SMILES:	Cc1cnc(C(=O)O)cn1
Mol. weight [g/mol]:	138.12
CAS:	5521-55-1

Physical Properties

Property code	Value	Unit	Source
hsub	100.90 ± 1.50	kJ/mol	NIST Webbook
log10ws	-1.54		Crippen Method
logp	0.483		Crippen Method
mcvol	99.040	ml/mol	McGowan Method
tt	440.35	K	Solubility Determination and Thermodynamic Mixing Properties of 5-Methyl-2-pyrazinecarboxylic Acid in Different Solvents

Sources

Solubility Determination and Thermodynamic Mixing Properties of 5-Methyl-2-pyrazinecarboxylic Acid in Different Solvents:	https://www.doi.org/10.1021/acs.jced.9b00406
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5521551&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hsub:	Enthalpy of sublimation at standard conditions

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