Trigonelline

Other names:	Pyridinium, 3-carboxy-1-methyl-, hydroxide, inner salt
	Betaine nicotinate
	Caffearine
	Coffearin
	Coffearine
	Gynesine
	Trigenolline
	Betain nicotinate
	3-Carboxy-1-methylpyridinium hydroxide inner salt
	N-Methylnicotinate
	N-Methylnicotinic acid
	N'-Methylnicotinic acid
	Nicotinic acid N-methylbetaine
	Trigonellin
	1-methylpyridinio-3-carboxylate
Inchi:	InChI=1S/C7H7NO2/c1-8-4-2-3-6(5-8)7(9)10/h2-5H,1H3
InchiKey:	WWNNZCOKKKDOPX-UHFFFAOYSA-N
Formula:	C7H7NO2
SMILES:	C[n+]1cccc(C(=O)[O-])c1
Mol. weight [g/mol]:	137.14
CAS:	535-83-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.96		Crippen Method
logp	-1.125		Crippen Method
mcvol	103.150	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C535831&Units=SI

Legend

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