3,4-PYRIDINEDICARBOXYLIC ACID

Other names:	Chinchomeronic acid
	Cinchomeronic acid
	Pyridine-3,4-dicarboxylic acid
Inchi:	InChI=1S/C7H5NO4/c9-6(10)4-1-2-8-3-5(4)7(11)12/h1-3H,(H,9,10)(H,11,12)
InchiKey:	MUYSADWCWFFZKR-UHFFFAOYSA-N
Formula:	C7H5NO4
SMILES:	O=C(O)c1ccncc1C(=O)O
Mol. weight [g/mol]:	167.12

Physical Properties

Property code	Value	Unit	Source
hf	-579.22	kJ/mol	Cheméo Relay (1.0)
ie	10.03	eV	Cheméo Relay (1.0)
log10ws	-1.11		Cheméo Relay (1.0)
logp	0.478		Crippen Method
mcvol	110.590	ml/mol	McGowan Method
tf	497.36	K	Cheméo Relay (1.0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C490119&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation at standard conditions
ie:	Ionization energy

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point