

2,5-Pyridinedicarboxylic acid

Other names:	Pyridine-2,5-dicarboxylic acid Pyridinedicarboxylic acid-(2,5) isocinchomeric acid
Inchi:	InChI=1S/C7H5NO4/c9-6(10)4-1-2-5(7(11)12)8-3-4/h1-3H,(H,9,10)(H,11,12)
InchiKey:	LVPMIMZXDYBCDF-UHFFFAOYSA-N
Formula:	C7H5NO4
SMILES:	O=C(O)c1ccc(C(=O)O)nc1
Mol. weight [g/mol]:	167.12
CAS:	100-26-5

Physical Properties

Property code	Value	Unit	Source
hsub	163.60 ± 2.70	kJ/mol	NIST Webbook
log10ws	-1.36		Crippen Method
logp	0.478		Crippen Method
mvol	110.590	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	194.40	kJ/mol	492.00	Thermochemical and Theoretical Studies of Dimethylpyridine-2,6-dicarboxylate and Pyridine-2,3-, Pyridine-2,5-, and Pyridine-2,6-dicarboxylic Acids

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C100265&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemical and Theoretical Studies of Dimethylpyridine-2,6-dicarboxylate and Pyridine-2,3-, Pyridine-2,5-, and Pyridine-2,6-dicarboxylic Acids: <https://www.doi.org/10.1021/je049586l>

Legend

hsub: Enthalpy of sublimation at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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