2,6-Pyridinedicarboxylic acid, dimethyl ester

Other names:	Dimethyl pyridine-2,6-dicarboxylate
	Pyridine-2,6-dicarboxylic acid dimethyl ester
	dimethyl 2,6-pyridinedicarboxylate
	dimethyl pyridine-2,6-carboxylate
Inchi:	InChI=1S/C9H9NO4/c1-13-8(11)6-4-3-5-7(10-6)9(12)14-2/h3-5H,1-2H3
InchiKey:	SNQQJEJPJMXYTR-UHFFFAOYSA-N
Formula:	C9H9NO4
SMILES:	COC(=O)c1cccc(C(=O)OC)n1
Mol. weight [g/mol]:	195.17
CAS:	5453-67-8

Physical Properties

Property code	Value	Unit	Source
hsub	113.50 ± 3.80	kJ/mol	NIST Webbook
log10ws	-1.72		Crippen Method
logp	0.655		Crippen Method
mcvol	138.770	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	130.00	kJ/mol	385.00	Thermochemical and Theoretical Studies of Dimethylpyridine-2,6-dicarboxylate and Pyridine-2,3-, Pyridine-2,5-, and Pyridine-2,6-dicarboxylic Acids

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5453678&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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