2,3-pyridinedicarboxylic acid

Other names: quinolinic acid
Inchi: InChI=1S/C7H5NO4/c9-6(10)4-2-1-3-8-5(4)7(11)12/h1-3H,(H,9,10)(H,11,12)
InchiKey: GJAWHXHKYYXBSV-UHFFFAOYSA-N
Formula: C7H5NO4
SMILES: O=C(O)c1cccnc1C(=O)O
Mol. weight [g/mol]: 167.12

Physical Properties

Property code	Value	Unit	Source
hf	-580.19	kJ/mol	Cheméo Relay (1.0)
ie	9.63	eV	Cheméo Relay (1.0)
log10ws	-1.04		Cheméo Relay (1.0)
logp	0.478		Crippen Method
mcvol	110.590	ml/mol	McGowan Method
tb	566.48	K	Cheméo Relay (1.0)
tc	887.00	K	Cheméo Relay (1.0)
tf	459.33	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

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

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):

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point