3-AMINOISONICOTINIC ACID

Other names: 4-Pyridinecarboxylic acid, 3-amino-
Inchi: InChI=1S/C6H6N2O2/c7-5-3-8-2-1-4(5)6(9)10/h1-3H,7H2,(H,9,10)
InchiKey: FYEQKMAVRYRMBL-UHFFFAOYSA-N
Formula: C6H6N2O2
SMILES: Nc1cnccc1C(=O)O
Mol. weight [g/mol]: 138.13

Physical Properties

Property code	Value	Unit	Source
hf	-240.20	kJ/mol	Cheméo Relay (1.0)
ie	9.03	eV	Cheméo Relay (1.0)
log10ws	-1.65		Cheméo Relay (1.0)
logp	0.362		Crippen Method
mcvol	99.040	ml/mol	McGowan Method
tf	550.59	K	Cheméo Relay (1.0)

Sources

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):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7579206&Units=SI

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