

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

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