6-AMINONICOTINAMIDE

Other names:	3-Pyridinecarboxamide, 6-amino- 2-Amino-5-carbamoylpyridine Nicotinamide, 6-amino- FDA 0121 NSC 21206 U-8774 6-Amino-nicotinsaeureamid 6-Aminonicotinic acid amide 6-Aminonikotinsaeureamid 6-AN 6-ANA SR 4388 6-Amino-3-pyridinecarboxamide
Inchi:	InChI=1S/C6H7N3O/c7-5-2-1-4(3-9-5)6(8)10/h1-3H,(H2,7,9)(H2,8,10)
InchiKey:	ZLWYEPMDOUQDBW-UHFFFAOYSA-N
Formula:	C6H7N3O
SMILES:	NC(=O)c1ccc(N)nc1
Mol. weight [g/mol]:	137.14

Physical Properties

Property code	Value	Unit	Source
hf	-99.96	kJ/mol	Cheméo Relay (1.0)
ie	8.59	eV	Cheméo Relay (1.0)
log10ws	-1.53		Cheméo Relay (1.0)
logp	-0.237		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
tb	577.55	K	Cheméo Relay (1.0)
tf	445.12	K	Cheméo Relay (1.0)

Sources

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=C329895&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tf:	Normal melting (fusion) point