

2-HYDROXYNICOTINIC ACID

Other names:	2-Hydroxynicotinic acid 1,2-dihydro-2-oxonicotinic acid
Inchi:	InChI=1S/C6H5NO3/c8-5-4(6(9)10)2-1-3-7-5/h1-3H,(H,7,8)(H,9,10)
InchiKey:	UEYQJQVBUVAELZ-UHFFFAOYSA-N
Formula:	C6H5NO3
SMILES:	O=C(O)c1cccnc1O
Mol. weight [g/mol]:	139.11

Physical Properties

Property code	Value	Unit	Source
hf	-463.41	kJ/mol	Cheméo Relay (1.0)
hsub	128.30 ± 5.10	kJ/mol	NIST Webbook
hvap	92.47	kJ/mol	Cheméo Relay (1.0)
ie	9.09	eV	Cheméo Relay (1.0)
log10ws	-1.64		Cheméo Relay (1.0)
logp	0.485		Crippen Method
mcvol	94.930	ml/mol	McGowan Method
tb	537.72	K	Cheméo Relay (1.0)
tc	852.94	K	Cheméo Relay (1.0)
tf	495.88	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	125.40 ± 5.00	kJ/mol	447.00	NIST Webbook

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=C609712&Units=SI>

Legend

hf:	Enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization 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

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