

5-CHLORO-6-HYDROXYNICOTINIC ACID

Inchi:	InChI=1S/C6H4ClNO3/c7-4-1-3(6(10)11)2-8-5(4)9/h1-2H,(H,8,9)(H,10,11)
InchiKey:	OLTRUTPHSBQWAZ-UHFFFAOYSA-N
Formula:	C6H4ClNO3
SMILES:	O=C(O)c1cnc(O)c(Cl)c1
Mol. weight [g/mol]:	173.56

Physical Properties

Property code	Value	Unit	Source
hf	-490.25	kJ/mol	Cheméo Relay (1.0)
hsub	151.30 ± 2.80	kJ/mol	NIST Webbook
log10ws	-1.92		Cheméo Relay (1.0)
logp	1.139		Crippen Method
mcvol	107.170	ml/mol	McGowan Method
tf	521.08	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	149.10 ± 2.60	kJ/mol	472.00	NIST Webbook

Sources

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=C54127638&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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