1-Methyl-5-fluorouracil

Inchi:	InChI=1S/C5H5FN2O2/c1-8-2-3(6)4(9)7-5(8)10/h2H,1H3,(H,7,9,10)
InchiKey:	PPCVYQHUOMISIG-UHFFFAOYSA-N
Formula:	C5H5FN2O2
SMILES:	Cn1cc(F)c(=O)[nH]c1=O
Mol. weight [g/mol]:	144.10
CAS:	155-16-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.15		Crippen Method
logp	-1.269		Crippen Method
mcvol	91.020	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	116.00 ± 2.00	kJ/mol	402.00	NIST Webbook
hsubt	126.00 ± 8.00	kJ/mol	497.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C155168&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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