1,2-DIHYDRO-4-METHOXYMETHYL-6-METHYL-2-O

Other names: Pyridine-3-carbonitrile, 1,2-dihydro-4-(methoxymethyl)-6-methyl-2-oxo-
4-(Methoxymethyl)-6-methyl-2-oxo-1,2-dihydro-3-pyridinecarbonitrile
3-Cyano-4-methoxymethyl-6-methyl-(2-pyridone)
1,2-Dihydro-4-methoxymethyl-6-methyl-2-oxo-3-pyridinecarbonitrile
3-Pyridinecarbonitrile, 1,2-dihydro-4-(methoxymethyl)-6-methyl-2-oxo-
2-Methyl-4-methoxymethyl-5-cyano-6-hydroxypyridine
5-Cyano-6-hydroxy-2-methyl-4-(methoxymethyl)pyridine
Inchi: InChI=1S/C9H10N2O2/c1-6-3-7(5-13-2)8(4-10)9(12)11-6/h3H,5H2,1-2H3,(H,11,12)
InchiKey: KLNRUMOPNATILS-UHFFFAOYSA-N
Formula: C9H10N2O2
SMILES: COCc1cc(C)[nH]c(=O)c1C#N
Mol. weight [g/mol]: 178.19

Physical Properties

Property code	Value	Unit	Source
logp	0.219		Crippen Method
mcvol	137.010	ml/mol	McGowan Method
ss	269.23	J/mol×K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	211.76	J/mol×K	298.15	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=C6339384&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cps:	Solid phase heat capacity
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ss:	Solid phase molar entropy at standard conditions