3-Cyano-4-methoxymethyl-5-nitro-6-methyl-(2-pyr

Inchi: InChI=1S/C9H9N3O4/c1-5-8(12(14)15)7(4-16-2)6(3-10)9(13)11-5/h4H2,1-2H3,(H,11,13)
InchiKey: FDZPYSHPLURJEA-UHFFFAOYSA-N
Formula: C9H9N3O4
SMILES: COCc1c(C#N)c(O)nc(C)c1[N+](=O)[O-]
Mol. weight [g/mol]: 223.19
CAS: 6281-75-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.65		Crippen Method
logp	1.022		Crippen Method
mcvol	154.430	ml/mol	McGowan Method
ss	323.69	J/mol×K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	275.80	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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6281750&Units=SI

Legend

cps:	Solid phase heat capacity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ss:	Solid phase molar entropy at standard conditions