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
af	0.7905		Cheméo Relay (1.0)
gf	141.79	kJ/mol	Cheméo Relay (1.0, beta)
hf	-128.01	kJ/mol	Cheméo Relay (1.0)
hvap	100.06	kJ/mol	Cheméo Relay (1.0)
ie	9.26	eV	Cheméo Relay (1.0)
log10ws	-2.62		Cheméo Relay (1.0)
logp	1.022		Crippen Method
mcvol	154.430	ml/mol	McGowan Method
pc	3343.07	kPa	Cheméo Relay (1.0, beta)
ss	323.69	J/mol×K	NIST Webbook
tb	590.14	K	Cheméo Relay (1.0)
tc	884.75	K	Cheméo Relay (1.0)
tf	482.55	K	Cheméo Relay (1.0)
vc	0.534	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	275.80	J/mol×K	298.15	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6281750&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	https://www.chemeo.com
Cheméo Relay (1.0, beta):	https://www.chemeo.com
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
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
pc:	Critical Pressure
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume