5-IMIDAZOLIC ACID, 4-NITRO-, METHYL(ESTER)

Other names: Imidazole-4-carboxylic acid, 5-nitro-, methyl ester
Inchi: InChI=1S/C5H5N3O4/c1-12-5(9)3-4(8(10)11)7-2-6-3/h2H,1H3,(H,6,7)
InchiKey: YGTWILAKCGDEML-UHFFFAOYSA-N
Formula: C5H5N3O4
SMILES: COC(=O)c1[nH]cnc1[N+](=O)[O-]
Mol. weight [g/mol]: 171.11

Physical Properties

Property code	Value	Unit	Source
hf	-184.45	kJ/mol	Cheméo Relay (1.0)
hvap	76.23	kJ/mol	Cheméo Relay (1.0)
ie	9.48	eV	Cheméo Relay (1.0)
log10ws	-2.79		Cheméo Relay (1.0)
logp	-0.377		Crippen Method
mcvol	106.670	ml/mol	McGowan Method
tf	414.56	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20271209&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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
tf:	Normal melting (fusion) point