2-FURANCARBOXALDEHYDE, 5-NITRO-, OXIME

Other names: 2-Furancarboxaldehyde, 5-nitro-, oxime
2-Furaldehyde, 5-nitro-, oxime
2-Furaldoxime, 5-nitro-
5-Nitro-2-furaldehyde oxime
USAF EA-5

Inchi: InChI=1S/C5H4N2O4/c8-6-3-4-1-2-5(11-4)7(9)10/h1-3,8H

InchiKey: PTBKFATYSVLSSD-UHFFFAOYSA-N

Formula: C5H4N2O4

SMILES: O=[N+]([O-])c1ccc(C=NO)o1

Mol. weight [g/mol]: 156.10

Physical Properties

Property code	Value	Unit	Source
hf	-46.66	kJ/mol	Cheméo Relay (1.0)
log10ws	-1.78		Cheméo Relay (1.0)
logp	0.996		Crippen Method
mcvol	96.690	ml/mol	McGowan Method
tf	385.21	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C555157&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

Cheméo Relay (1.0):

Legend

hf: Enthalpy of formation at standard conditions

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point