METHYL 5-NITRO-2-FURANCARBOXYLATE

Other names:	Methyl 5-nitro-2-furoate
	2-Furancarboxylic acid, 5-nitro-, methyl ester
	2-Furoic acid, 5-nitro-, methyl ester
	Methyl nitrofuroate
	Methyl 5-nitrofuroate
	Methyl 5-nitropyromucate
	Methyl 5'-nitropyromucate
	5-Nitro-2-furoic acid methyl ester
	NSC 6457
	Methyl 5-nitro-2-furylcarboxylate
Inchi:	InChI=1S/C6H5NO5/c1-11-6(8)4-2-3-5(12-4)7(9)10/h2-3H,1H3
InchiKey:	UTLKCGPAJUYGOM-UHFFFAOYSA-N
Formula:	C6H5NO5
SMILES:	COC(=O)c1ccc([N+](=O)[O-])o1
Mol. weight [g/mol]:	171.11

Physical Properties

Property code	Value	Unit	Source
chs	-2605.00 ± 0.40	kJ/mol	NIST Webbook
hf	-367.00 ± 2.00	kJ/mol	NIST Webbook
hfs	-471.10 ± 0.40	kJ/mol	NIST Webbook
hvap	73.70	kJ/mol	Cheméo Relay (1.0)
ie	9.86	eV	Cheméo Relay (1.0)
log10ws	-2.41		Cheméo Relay (1.0)
logp	0.974		Crippen Method
mcvol	106.670	ml/mol	McGowan Method
tb	520.98	K	Cheméo Relay (1.0)
tf	350.05	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	104.00 ± 2.00	kJ/mol	303.00	NIST Webbook

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1874233&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

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point