5-NITROFURFURYLIDENE DIACETATE

Other names:	5-Nitro-2-furaldehyde diacetate
	5-Nitrofurfurylidene diacetate
	5-Nitrofurfural diacetate
	Methanediol, (5-nitro-2-furanyl)-, diacetate
	Methanediol, (5-nitro-2-furanyl)-, diacetate (ester)
	Nitrofuraldehyde diacetate
	2-Furanmethanediol, 5-nitro-, diacetate
	5-Nitro-2-furancarboxaldehyde diacetate
	5-Nitro-2-furanmethandiol diacetate
	5-Nitro-2-furanmethanediol diacetate
	5-Nitro-2-furfural diacetate
	5-Nitro-2-furfuraldehyde diacetate
	5-Nitrofuraldehyde diacetate
	Methanediol, 1-(5-nitro-2-furanyl)-, 1,1-diacetate
	NSC 5411
Inchi:	InChI=1S/C9H9NO7/c1-5(11)15-9(16-6(2)12)7-3-4-8(17-7)10(13)14/h3-4,9H,1-2H3
InchiKey:	HSXKWKJCZNRMJO-UHFFFAOYSA-N
Formula:	C9H9NO7
SMILES:	CC(=O)OC(OC(C)=O)c1ccc([N+](=O)[O-])o1
Mol. weight [g/mol]:	243.17

Physical Properties

Property code	Value	Unit	Source
chs	-3930.00 ± 0.80	kJ/mol	NIST Webbook
hf	-772.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-897.90 ± 0.80	kJ/mol	NIST Webbook
logp	1.313		Crippen Method
mcvol	156.380	ml/mol	McGowan Method
tf	325.22	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	126.00 ± 3.00	kJ/mol	288.00	NIST Webbook

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92557&Units=SI

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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point