5-Nitro-2-acetoxy-2,5-dihydrofurfural diacetate

Inchi: InChI=1S/C11H13NO9/c1-6(13)18-10(19-7(2)14)11(20-8(3)15)5-4-9(21-11)12(16)17/h4-5
InchiKey: OQQARHHKPBGAGA-UHFFFAOYSA-N
Formula: C11H13NO9
SMILES: CC(=O)OC(OC(C)=O)C1(OC(C)=O)C=CC([N+](=O)[O-])O1
Mol. weight [g/mol]: 303.22
CAS: 75631-81-1

Physical Properties

Property code	Value	Unit	Source
chs	-4812.00 ± 2.00	kJ/mol	NIST Webbook
gf	-659.72	kJ/mol	Joback Method
hf	-1285.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-1374.00 ± 2.00	kJ/mol	NIST Webbook
hfus	38.35	kJ/mol	Joback Method
hsub	89.00 ± 2.00	kJ/mol	NIST Webbook
hvap	87.35	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	-0.113		Crippen Method
mcvol	196.300	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
tb	868.31	K	Joback Method
tc	1103.54	K	Joback Method
tf	616.71	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.98	J/mol×K	868.31	Joback Method
cpg	614.32	J/mol×K	907.51	Joback Method
cpg	626.17	J/mol×K	946.72	Joback Method
cpg	637.63	J/mol×K	985.92	Joback Method
cpg	648.78	J/mol×K	1025.13	Joback Method
cpg	659.72	J/mol×K	1064.33	Joback Method

cpg	670.53	J/mol×K	1103.54	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75631811&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume