

2-Nitrotoluene-«alpha»,«alpha»-diol diacetate

Other names:	o-Nitrobenzal diacetate 2-Nitrobenzaldehyde diacetate Methanediol, (2-nitrophenyl)-, diacetate Toluene-alpha,alpha-diol, o-nitro-, diacetate 2-nitrobenzylidene di(acetate)
Inchi:	InChI=1S/C11H11NO6/c1-7(13)17-11(18-8(2)14)9-5-3-4-6-10(9)12(15)16/h3-6,11H,1-2H
InchiKey:	PMZHONATLZBKIL-UHFFFAOYSA-N
Formula:	C11H11NO6
SMILES:	CC(=O)OC(OC(C)=O)c1cccc1[N+](=O)[O-]
Mol. weight [g/mol]:	253.21
CAS:	6345-63-7

Physical Properties

Property code	Value	Unit	Source
gf	-290.21	kJ/mol	Joback Method
hf	-550.95	kJ/mol	Joback Method
hfus	31.31	kJ/mol	Joback Method
hvap	77.53	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	1.720		Crippen Method
mcvol	174.390	ml/mol	McGowan Method
pc	2934.52	kPa	Joback Method
tb	786.72	K	Joback Method
tc	1025.73	K	Joback Method
tf	525.60	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.78	J/molxK	786.72	Joback Method
cpg	491.70	J/molxK	826.55	Joback Method
cpg	501.58	J/molxK	866.39	Joback Method
cpg	510.40	J/molxK	906.22	Joback Method

cpg	518.18	J/mol×K	946.06	Joback Method
cpg	524.93	J/mol×K	985.89	Joback Method
cpg	530.64	J/mol×K	1025.73	Joback Method

Sources

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=C6345637&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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

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