Acetamide, N-(3-nitrophenyl)-2-acetoxy-

Inchi: InChI=1S/C10H10N2O5/c1-7(13)17-6-10(14)11-8-3-2-4-9(5-8)12(15)16/h2-5H,6H2,1H3,(
InchiKey: FXPSKSZDZMYNHZ-UHFFFAOYSA-N
Formula: C10H10N2O5
SMILES: CC(=O)OCC(=O)Nc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 238.20

Physical Properties

Property code	Value	Unit	Source
gf	-101.80	kJ/mol	Joback Method
hf	-339.34	kJ/mol	Joback Method
hfus	36.15	kJ/mol	Joback Method
hvap	79.72	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	1.096		Crippen Method
mcvol	164.410	ml/mol	McGowan Method
pc	3348.98	kPa	Joback Method
rinpol	2056.00		NIST Webbook
tb	792.03	K	Joback Method
tc	1031.99	K	Joback Method
tf	559.76	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.45	J/mol×K	792.03	Joback Method
cpg	461.45	J/mol×K	832.02	Joback Method
cpg	470.50	J/mol×K	872.02	Joback Method
cpg	478.62	J/mol×K	912.01	Joback Method
cpg	485.83	J/mol×K	952.00	Joback Method
cpg	492.17	J/mol×K	992.00	Joback Method
cpg	497.65	J/mol×K	1031.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307096&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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