Acetic acid, 3-nitrophenyl ester

Inchi: InChI=1S/C8H7NO4/c1-6(10)13-8-4-2-3-7(5-8)9(11)12/h2-5H,1H3
InchiKey: HRMRLUUZPLAPAS-UHFFFAOYSA-N
Formula: C8H7NO4
SMILES: CC(=O)Oc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 181.15
CAS: 1523-06-4

Physical Properties

Property code	Value	Unit	Source
gf	-79.11	kJ/mol	Joback Method
hf	-238.95	kJ/mol	Joback Method
hfus	24.28	kJ/mol	Joback Method
hvap	62.09	kJ/mol	Joback Method
ie	9.40 ± 0.20	eV	NIST Webbook
log10ws	-2.44		Crippen Method
logp	1.520		Crippen Method
mcvol	124.680	ml/mol	McGowan Method
pc	3848.31	kPa	Joback Method
rinpol	1348.00		NIST Webbook
rinpol	1348.00		NIST Webbook
tb	642.23	K	Joback Method
tc	889.97	K	Joback Method
tf	434.63	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.26	J/mol×K	642.23	Joback Method
cpg	308.88	J/mol×K	683.52	Joback Method
cpg	318.68	J/mol×K	724.81	Joback Method
cpg	327.67	J/mol×K	766.10	Joback Method
cpg	335.88	J/mol×K	807.39	Joback Method
cpg	343.31	J/mol×K	848.68	Joback Method

cpg	349.99	J/mol×K	889.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1523064&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
ie:	Ionization energy
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