Benzeneethanol, 3-nitro-, acetate (ester)

Other names:	Acetic acid, 2-(3-nitrophenyl)ethyl ester
	m-nitrophenethyl acetate
Inchi:	InChI=1S/C10H11NO4/c1-8(12)15-6-5-9-3-2-4-10(7-9)11(13)14/h2-4,7H,5-6H2,1H3
InchiKey:	DHCRSUDNZBCHMQ-UHFFFAOYSA-N
Formula:	C10H11NO4
SMILES:	CC(=O)OCCc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	209.20
CAS:	68527-46-8

Physical Properties

Property code	Value	Unit	Source
gf	-62.27	kJ/mol	Joback Method
hf	-280.23	kJ/mol	Joback Method
hfus	29.46	kJ/mol	Joback Method
hvap	66.54	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	1.700		Crippen Method
mcvol	152.860	ml/mol	McGowan Method
pc	3072.75	kPa	Joback Method
rinpol	1718.00		NIST Webbook
rinpol	1718.00		NIST Webbook
tb	687.99	K	Joback Method
tc	925.31	K	Joback Method
tf	457.17	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.14	J/mol×K	687.99	Joback Method
cpg	407.29	J/mol×K	727.54	Joback Method
cpg	418.53	J/mol×K	767.10	Joback Method
cpg	428.88	J/mol×K	806.65	Joback Method
cpg	438.36	J/mol×K	846.20	Joback Method

cpg	446.99	J/mol×K	885.75	Joback Method
cpg	454.81	J/mol×K	925.31	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=C68527468&Units=SI

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