Acetic acid, (4-fluoro-3-nitrophenyl)methyl ester

Inchi: InChI=1S/C9H8FNO4/c1-6(12)15-5-7-2-3-8(10)9(4-7)11(13)14/h2-4H,5H2,1H3
InchiKey: OHFZUFHGTANCOR-UHFFFAOYSA-N
Formula: C9H8FNO4
SMILES: CC(=O)OCc1ccc(F)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 213.16

Physical Properties

Property code	Value	Unit	Source
gf	-275.13	kJ/mol	Joback Method
hf	-467.17	kJ/mol	Joback Method
hfus	29.56	kJ/mol	Joback Method
hvap	64.16	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	1.797		Crippen Method
mcvol	140.540	ml/mol	McGowan Method
pc	3199.16	kPa	Joback Method
rinpol	1602.00		NIST Webbook
tb	669.36	K	Joback Method
tc	901.37	K	Joback Method
tf	459.01	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.57	J/mol×K	669.36	Joback Method
cpg	363.26	J/mol×K	708.03	Joback Method
cpg	373.17	J/mol×K	746.70	Joback Method
cpg	382.32	J/mol×K	785.36	Joback Method
cpg	390.73	J/mol×K	824.03	Joback Method
cpg	398.40	J/mol×K	862.70	Joback Method
cpg	405.34	J/mol×K	901.37	Joback Method

Sources

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=U368234&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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