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

Inchi: InChI=1S/C8H6FNO4/c9-7-2-1-6(4-14-5-11)3-8(7)10(12)13/h1-3,5H,4H2
InchiKey: FJGKHWVRZIWVIY-UHFFFAOYSA-N
Formula: C8H6FNO4
SMILES: O=COCc1ccc(F)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 199.14

Physical Properties

Property code	Value	Unit	Source
gf	-254.15	kJ/mol	Joback Method
hf	-419.53	kJ/mol	Joback Method
hfus	27.66	kJ/mol	Joback Method
hvap	61.91	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	1.407		Crippen Method
mcvol	126.450	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
rinpol	1551.00		NIST Webbook
rinpol	1551.00		NIST Webbook
tb	641.27	K	Joback Method
tc	872.87	K	Joback Method
tf	439.81	K	Joback Method
vc	0.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.19	J/mol×K	641.27	Joback Method
cpg	315.78	J/mol×K	679.87	Joback Method
cpg	324.69	J/mol×K	718.47	Joback Method
cpg	332.92	J/mol×K	757.07	Joback Method
cpg	340.50	J/mol×K	795.67	Joback Method
cpg	347.43	J/mol×K	834.27	Joback Method
cpg	353.72	J/mol×K	872.87	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=U368233&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