Formic acid, 2-(3-nitrophenyl)ethyl ester

Inchi: InChI=1S/C9H9NO4/c11-7-14-5-4-8-2-1-3-9(6-8)10(12)13/h1-3,6-7H,4-5H2
InchiKey: QSHDHOFHYIOUTH-UHFFFAOYSA-N
Formula: C9H9NO4
SMILES: O=COCCc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 195.17

Physical Properties

Property code	Value	Unit	Source
gf	-41.29	kJ/mol	Joback Method
hf	-232.59	kJ/mol	Joback Method
hfus	27.56	kJ/mol	Joback Method
hvap	64.29	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	1.310		Crippen Method
mcvol	138.770	ml/mol	McGowan Method
pc	3472.45	kPa	Joback Method
rinpol	1659.00		NIST Webbook
rinpol	1659.00		NIST Webbook
tb	659.90	K	Joback Method
tc	897.04	K	Joback Method
tf	437.97	K	Joback Method
vc	0.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.00	J/mol×K	659.90	Joback Method
cpg	358.18	J/mol×K	699.42	Joback Method
cpg	368.52	J/mol×K	738.95	Joback Method
cpg	378.06	J/mol×K	778.47	Joback Method
cpg	386.81	J/mol×K	818.00	Joback Method
cpg	394.80	J/mol×K	857.52	Joback Method
cpg	402.04	J/mol×K	897.04	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=U368222&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