Formic acid, 2-(4-nitrophenoxy)ethyl ester

Inchi: InChI=1S/C9H9NO5/c11-7-14-5-6-15-9-3-1-8(2-4-9)10(12)13/h1-4,7H,5-6H2
InchiKey: VICWPMCACVBXQW-UHFFFAOYSA-N
Formula: C9H9NO5
SMILES: O=COCCOc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 211.17

Physical Properties

Property code	Value	Unit	Source
gf	-146.29	kJ/mol	Joback Method
hf	-364.81	kJ/mol	Joback Method
hfus	28.74	kJ/mol	Joback Method
hvap	66.70	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	1.147		Crippen Method
mcvol	144.640	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
rinpol	1860.00		NIST Webbook
tb	682.32	K	Joback Method
tc	915.95	K	Joback Method
tf	460.20	K	Joback Method
vc	0.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.09	J/mol×K	682.32	Joback Method
cpg	381.09	J/mol×K	721.26	Joback Method
cpg	391.28	J/mol×K	760.20	Joback Method
cpg	400.65	J/mol×K	799.14	Joback Method
cpg	409.20	J/mol×K	838.08	Joback Method
cpg	416.95	J/mol×K	877.01	Joback Method
cpg	423.88	J/mol×K	915.95	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=U368925&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