Carbonic acid, ethyl 2-nitro-5-fluorophenyl ester

Inchi: InChI=1S/C9H8FNO5/c1-2-15-9(12)16-8-5-6(10)3-4-7(8)11(13)14/h3-5H,2H2,1H3
InchiKey: VBGZJAOJZNJVOU-UHFFFAOYSA-N
Formula: C9H8FNO5
SMILES: CCOC(=O)Oc1cc(F)ccc1[N+](=O)[O-]
Mol. weight [g/mol]: 229.16

Physical Properties

Property code	Value	Unit	Source
gf	-380.13	kJ/mol	Joback Method
hf	-599.39	kJ/mol	Joback Method
hfus	30.75	kJ/mol	Joback Method
hvap	66.57	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.269		Crippen Method
mcvol	146.410	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
rinpol	1525.00		NIST Webbook
tb	691.78	K	Joback Method
tc	920.56	K	Joback Method
tf	481.24	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.62	J/mol×K	691.78	Joback Method
cpg	386.16	J/mol×K	729.91	Joback Method
cpg	395.92	J/mol×K	768.04	Joback Method
cpg	404.91	J/mol×K	806.17	Joback Method
cpg	413.12	J/mol×K	844.30	Joback Method
cpg	420.54	J/mol×K	882.43	Joback Method
cpg	427.16	J/mol×K	920.56	Joback Method

Sources

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=U357920&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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