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

Inchi: InChI=1S/C11H12FNO5/c1-7(2)6-17-11(14)18-10-5-8(12)3-4-9(10)13(15)16/h3-5,7H,6H2

InchiKey: DVGUIWXNVXRKLD-UHFFFAOYSA-N

Formula: C11H12FNO5

SMILES: CC(C)COC(=O)Oc1cc(F)ccc1[N+](=O)[O-]

Mol. weight [g/mol]: 257.22

Physical Properties

Property code	Value	Unit	Source
gf	-365.73	kJ/mol	Joback Method
hf	-645.95	kJ/mol	Joback Method
hfus	32.40	kJ/mol	Joback Method
hvap	70.63	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	2.905		Crippen Method
mcvol	174.590	ml/mol	McGowan Method
pc	2579.34	kPa	Joback Method
rinpol	1674.00		NIST Webbook
rinpol	1674.00		NIST Webbook
tb	737.10	K	Joback Method
tc	962.10	K	Joback Method
tf	488.78	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.45	J/mol×K	737.10	Joback Method
cpg	489.41	J/mol×K	774.60	Joback Method
cpg	500.46	J/mol×K	812.10	Joback Method
cpg	510.60	J/mol×K	849.60	Joback Method
cpg	519.82	J/mol×K	887.10	Joback Method
cpg	528.13	J/mol×K	924.60	Joback Method
cpg	535.53	J/mol×K	962.10	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=U357835&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