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

Inchi: InChI=1S/C18H16FNO6/c1-11(2)10-25-17(21)12-4-3-5-13(8-12)18(22)26-16-9-14(19)6-7

InchiKey: GTXBMHNSCWOICF-UHFFFAOYSA-N

Formula: C18H16FNO6

SMILES: CC(C)COC(=O)c1cccc(C(=O)Oc2cc(F)ccc2[N+](=O)[O-])c1

Mol. weight [g/mol]: 361.32

Physical Properties

Property code	Value	Unit	Source
gf	-332.93	kJ/mol	Joback Method
hf	-677.95	kJ/mol	Joback Method
hfus	45.78	kJ/mol	Joback Method
hvap	95.90	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	3.766		Crippen Method
mcvol	251.030	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
rinpol	2699.00		NIST Webbook
rinpol	2699.00		NIST Webbook
tb	982.79	K	Joback Method
tc	1226.94	K	Joback Method
tf	656.54	K	Joback Method
vc	0.970	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.57	J/mol×K	982.79	Joback Method
cpg	775.87	J/mol×K	1023.48	Joback Method
cpg	783.78	J/mol×K	1064.17	Joback Method
cpg	790.32	J/mol×K	1104.87	Joback Method
cpg	795.54	J/mol×K	1145.56	Joback Method
cpg	799.46	J/mol×K	1186.25	Joback Method
cpg	802.11	J/mol×K	1226.94	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U344417&Units=SI

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