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

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

InchiKey: QBUGJNLRCFEPNO-UHFFFAOYSA-N

Formula: C18H16FNO6

SMILES: CCCCOC(=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	-330.49	kJ/mol	Joback Method
hf	-672.67	kJ/mol	Joback Method
hfus	49.31	kJ/mol	Joback Method
hvap	96.29	kJ/mol	Joback Method
log10ws	-6.04		Crippen Method
logp	3.910		Crippen Method
mcvol	251.030	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpol	2749.00		NIST Webbook
rinpol	2749.00		NIST Webbook
tb	983.23	K	Joback Method
tc	1224.77	K	Joback Method
tf	671.54	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.10	J/mol×K	983.23	Joback Method
cpg	775.38	J/mol×K	1023.49	Joback Method
cpg	783.31	J/mol×K	1063.74	Joback Method
cpg	789.92	J/mol×K	1104.00	Joback Method
cpg	795.24	J/mol×K	1144.26	Joback Method
cpg	799.31	J/mol×K	1184.51	Joback Method
cpg	802.15	J/mol×K	1224.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344418&Units=SI
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

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