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

Inchi: InChI=1S/C23H26FNO6/c1-2-3-4-5-6-7-8-14-30-22(26)17-10-9-11-18(15-17)23(27)31-21

InchiKey: IGXVBPMOIKLZEX-UHFFFAOYSA-N

Formula: C23H26FNO6

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

Mol. weight [g/mol]: 431.45

Physical Properties

Property code	Value	Unit	Source
gf	-288.39	kJ/mol	Joback Method
hf	-775.87	kJ/mol	Joback Method
hfus	62.26	kJ/mol	Joback Method
hvap	107.42	kJ/mol	Joback Method
log10ws	-8.13		Crippen Method
logp	5.861		Crippen Method
mcvol	321.480	ml/mol	McGowan Method
pc	1322.31	kPa	Joback Method
rinpol	3283.00		NIST Webbook
tb	1097.63	K	Joback Method
tc	1344.75	K	Joback Method
tf	727.89	K	Joback Method
vc	1.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1056.77	J/mol×K	1097.63	Joback Method
cpg	1066.11	J/mol×K	1138.82	Joback Method
cpg	1073.90	J/mol×K	1180.00	Joback Method
cpg	1080.19	J/mol×K	1221.19	Joback Method
cpg	1085.04	J/mol×K	1262.37	Joback Method
cpg	1088.52	J/mol×K	1303.56	Joback Method
cpg	1090.67	J/mol×K	1344.75	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=U344424&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