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

Inchi: InChI=1S/C19H18FNO6/c1-2-3-4-10-26-18(22)13-6-5-7-14(11-13)19(23)27-17-12-15(20)

InchiKey: SMXUSYHMILNKBU-UHFFFAOYSA-N

Formula: C19H18FNO6

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

Mol. weight [g/mol]: 375.35

Physical Properties

Property code	Value	Unit	Source
gf	-322.07	kJ/mol	Joback Method
hf	-693.31	kJ/mol	Joback Method
hfus	51.90	kJ/mol	Joback Method
hvap	98.51	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	4.300		Crippen Method
mcvol	265.120	ml/mol	McGowan Method
pc	1786.37	kPa	Joback Method
rinpol	2849.00		NIST Webbook
rinpol	2849.00		NIST Webbook
tb	1006.11	K	Joback Method
tc	1246.87	K	Joback Method
tf	682.81	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.27	J/mol×K	1006.11	Joback Method
cpg	832.59	J/mol×K	1046.24	Joback Method
cpg	840.53	J/mol×K	1086.36	Joback Method
cpg	847.13	J/mol×K	1126.49	Joback Method
cpg	852.43	J/mol×K	1166.62	Joback Method
cpg	856.45	J/mol×K	1206.75	Joback Method
cpg	859.24	J/mol×K	1246.87	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=U344419&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