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

Inchi: InChI=1S/C22H24FNO6/c1-2-3-4-5-6-7-13-29-21(25)16-9-8-10-17(14-16)22(26)30-20-15

InchiKey: CTOFLIUHKKVPKA-UHFFFAOYSA-N

Formula: C22H24FNO6

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

Mol. weight [g/mol]: 417.43

Physical Properties

Property code	Value	Unit	Source
gf	-296.81	kJ/mol	Joback Method
hf	-755.23	kJ/mol	Joback Method
hfus	59.67	kJ/mol	Joback Method
hvap	105.19	kJ/mol	Joback Method
log10ws	-7.71		Crippen Method
logp	5.470		Crippen Method
mcvol	307.390	ml/mol	McGowan Method
pc	1419.71	kPa	Joback Method
rinpol	3180.00		NIST Webbook
rinpol	3180.00		NIST Webbook
tb	1074.75	K	Joback Method
tc	1318.75	K	Joback Method
tf	716.62	K	Joback Method
vc	1.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.76	J/mol×K	1074.75	Joback Method
cpg	1007.11	J/mol×K	1115.42	Joback Method
cpg	1014.96	J/mol×K	1156.08	Joback Method
cpg	1021.37	J/mol×K	1196.75	Joback Method
cpg	1026.38	J/mol×K	1237.42	Joback Method
cpg	1030.04	J/mol×K	1278.09	Joback Method
cpg	1032.41	J/mol×K	1318.75	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=U344423&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