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

Inchi: InChI=1S/C20H20FNO6/c1-13(2)5-4-10-27-19(23)14-6-3-7-15(11-14)20(24)28-18-12-16(
InchiKey: MFJXCJOKGOKSLM-UHFFFAOYSA-N
Formula: C20H20FNO6
SMILES: CC(C)CCCOC(=O)c1cccc(C(=O)Oc2cc(F)ccc2[N+](=O)[O-])c1
Mol. weight [g/mol]: 389.37

Physical Properties

Property code	Value	Unit	Source
gf	-316.09	kJ/mol	Joback Method
hf	-719.23	kJ/mol	Joback Method
hfus	50.96	kJ/mol	Joback Method
hvap	100.35	kJ/mol	Joback Method
log10ws	-6.63		Crippen Method
logp	4.546		Crippen Method
mcvol	279.210	ml/mol	McGowan Method
pc	1660.55	kPa	Joback Method
rinpol	2906.00		NIST Webbook
rinpol	2906.00		NIST Webbook
tb	1028.55	K	Joback Method
tc	1271.26	K	Joback Method
tf	679.08	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.33	J/mol×K	1028.55	Joback Method
cpg	890.66	J/mol×K	1069.00	Joback Method
cpg	898.54	J/mol×K	1109.45	Joback Method
cpg	905.01	J/mol×K	1149.90	Joback Method
cpg	910.11	J/mol×K	1190.36	Joback Method
cpg	913.89	J/mol×K	1230.81	Joback Method
cpg	916.37	J/mol×K	1271.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344420&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

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