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

Inchi: InChI=1S/C21H22FNO6/c1-2-3-4-5-6-12-28-20(24)15-8-7-9-16(13-15)21(25)29-19-14-17

InchiKey: XGUIFQNFYJKYPG-UHFFFAOYSA-N

Formula: C21H22FNO6

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

Mol. weight [g/mol]: 403.40

Physical Properties

Property code	Value	Unit	Source
gf	-305.23	kJ/mol	Joback Method
hf	-734.59	kJ/mol	Joback Method
hfus	57.08	kJ/mol	Joback Method
hvap	102.96	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	5.080		Crippen Method
mcvol	293.300	ml/mol	McGowan Method
pc	1528.27	kPa	Joback Method
rinpol	3075.00		NIST Webbook
rinpol	3075.00		NIST Webbook
tb	1051.87	K	Joback Method
tc	1293.81	K	Joback Method
tf	705.35	K	Joback Method
vc	1.143	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	939.14	J/mol×K	1051.87	Joback Method
cpg	948.49	J/mol×K	1092.19	Joback Method
cpg	956.40	J/mol×K	1132.52	Joback Method
cpg	962.89	J/mol×K	1172.84	Joback Method
cpg	968.03	J/mol×K	1213.17	Joback Method
cpg	971.85	J/mol×K	1253.49	Joback Method
cpg	974.39	J/mol×K	1293.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344422&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

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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