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

Inchi: InChI=1S/C17H14FNO6/c1-2-8-24-16(20)11-4-3-5-12(9-11)17(21)25-15-10-13(18)6-7-14

InchiKey: IJDVRCLUDMZETB-UHFFFAOYSA-N

Formula: C17H14FNO6

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

Mol. weight [g/mol]: 347.29

Physical Properties

Property code	Value	Unit	Source
gf	-338.91	kJ/mol	Joback Method
hf	-652.03	kJ/mol	Joback Method
hfus	46.72	kJ/mol	Joback Method
hvap	94.06	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	3.520		Crippen Method
mcvol	236.940	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
rinpol	2647.00		NIST Webbook
rinpol	2647.00		NIST Webbook
tb	960.35	K	Joback Method
tc	1203.51	K	Joback Method
tf	660.27	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.53	J/mol×K	960.35	Joback Method
cpg	718.73	J/mol×K	1000.88	Joback Method
cpg	726.60	J/mol×K	1041.40	Joback Method
cpg	733.19	J/mol×K	1081.93	Joback Method
cpg	738.50	J/mol×K	1122.46	Joback Method
cpg	742.57	J/mol×K	1162.99	Joback Method
cpg	745.43	J/mol×K	1203.51	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=U344416&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