Terephthalic acid, 2-(3-nitrophenyl)ethyl propyl ester

Inchi: InChI=1S/C19H19NO6/c1-2-11-25-18(21)15-6-8-16(9-7-15)19(22)26-12-10-14-4-3-5-17(
InchiKey: SVUDAXGUSNSEAI-UHFFFAOYSA-N
Formula: C19H19NO6
SMILES: CCCOC(=O)c1ccc(C(=O)OCCc2cccc([N+](=O)[O-])c2)cc1
Mol. weight [g/mol]: 357.36

Physical Properties

Property code	Value	Unit	Source
gf	-117.63	kJ/mol	Joback Method
hf	-485.73	kJ/mol	Joback Method
hfus	49.20	kJ/mol	Joback Method
hvap	98.67	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	3.561		Crippen Method
mcvol	263.350	ml/mol	McGowan Method
pc	1880.53	kPa	Joback Method
rinpol	3049.00		NIST Webbook
rinpol	3049.00		NIST Webbook
tb	1001.86	K	Joback Method
tc	1247.36	K	Joback Method
tf	669.70	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	818.17	J/mol×K	1001.86	Joback Method
cpg	828.01	J/mol×K	1042.78	Joback Method
cpg	836.44	J/mol×K	1083.69	Joback Method
cpg	843.51	J/mol×K	1124.61	Joback Method
cpg	849.27	J/mol×K	1165.52	Joback Method
cpg	853.77	J/mol×K	1206.44	Joback Method
cpg	857.04	J/mol×K	1247.36	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416105&Units=SI

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