Terephthalic acid, 3-nitro-4-methylbenzyl propyl ester

Inchi: InChI=1S/C19H19NO6/c1-3-10-25-18(21)15-6-8-16(9-7-15)19(22)26-12-14-5-4-13(2)17(
InchiKey: OPPSFJLGGGUUQK-UHFFFAOYSA-N
Formula: C19H19NO6
SMILES: CCCOC(=O)c1ccc(C(=O)OCc2ccc(C)c([N+](=O)[O-])c2)cc1
Mol. weight [g/mol]: 357.36

Physical Properties

Property code	Value	Unit	Source
gf	-127.26	kJ/mol	Joback Method
hf	-497.20	kJ/mol	Joback Method
hfus	48.82	kJ/mol	Joback Method
hvap	99.33	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	3.827		Crippen Method
mcvol	263.350	ml/mol	McGowan Method
pc	1856.31	kPa	Joback Method
rinpol	3023.00		NIST Webbook
tb	1006.84	K	Joback Method
tc	1253.08	K	Joback Method
tf	682.22	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.41	J/mol×K	1006.84	Joback Method
cpg	826.07	J/mol×K	1047.88	Joback Method
cpg	834.29	J/mol×K	1088.92	Joback Method
cpg	841.10	J/mol×K	1129.96	Joback Method
cpg	846.54	J/mol×K	1171.00	Joback Method
cpg	850.64	J/mol×K	1212.04	Joback Method
cpg	853.44	J/mol×K	1253.08	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=U416086&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