Terephthalic acid, isobutyl 2-(4-nitrophenoxy)ethyl ester

Inchi: InChI=1S/C20H21NO7/c1-14(2)13-28-20(23)16-5-3-15(4-6-16)19(22)27-12-11-26-18-9-7

InchiKey: QTANQCCZELAGTJ-UHFFFAOYSA-N

Formula: C20H21NO7

SMILES: CC(C)COC(=O)c1ccc(C(=O)OCCOc2ccc([N+](=O)[O-])cc2)cc1

Mol. weight [g/mol]: 387.38

Physical Properties

Property code	Value	Unit	Source
gf	-216.65	kJ/mol	Joback Method
hf	-643.87	kJ/mol	Joback Method
hfus	49.46	kJ/mol	Joback Method
hvap	102.92	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	3.643		Crippen Method
mcvol	283.310	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	3289.00		NIST Webbook
rinpol	3289.00		NIST Webbook
tb	1046.72	K	Joback Method
tc	1293.83	K	Joback Method
tf	688.20	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	900.01	J/mol×K	1046.72	Joback Method
cpg	908.49	J/mol×K	1087.90	Joback Method
cpg	915.31	J/mol×K	1129.09	Joback Method
cpg	920.49	J/mol×K	1170.27	Joback Method
cpg	924.04	J/mol×K	1211.46	Joback Method
cpg	926.02	J/mol×K	1252.64	Joback Method
cpg	926.43	J/mol×K	1293.83	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=U416090&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