Phthalic acid, 2-(4-nitrophenoxy)ethyl pentyl ester

Inchi: InChI=1S/C21H23NO7/c1-2-3-6-13-28-20(23)18-7-4-5-8-19(18)21(24)29-15-14-27-17-11

InchiKey: IUDXMMRWJGLIIY-UHFFFAOYSA-N

Formula: C21H23NO7

SMILES: CCCCCOC(=O)c1ccccc1C(=O)OCCOc1ccc([N+](=O)[O-])cc1

Mol. weight [g/mol]: 401.41

Physical Properties

Property code	Value	Unit	Source
gf	-205.79	kJ/mol	Joback Method
hf	-659.23	kJ/mol	Joback Method
hfus	55.57	kJ/mol	Joback Method
hvap	105.53	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	4.178		Crippen Method
mcvol	297.400	ml/mol	McGowan Method
pc	1580.97	kPa	Joback Method
rinpol	3532.00		NIST Webbook
rinpol	3532.00		NIST Webbook
tb	1070.04	K	Joback Method
tc	1316.24	K	Joback Method
tf	714.47	K	Joback Method
vc	1.143	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.68	J/mol×K	1070.04	Joback Method
cpg	966.08	J/mol×K	1111.07	Joback Method
cpg	972.81	J/mol×K	1152.11	Joback Method
cpg	977.89	J/mol×K	1193.14	Joback Method
cpg	981.36	J/mol×K	1234.18	Joback Method
cpg	983.26	J/mol×K	1275.21	Joback Method
cpg	983.60	J/mol×K	1316.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382575&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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