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

Inchi: InChI=1S/C22H25NO7/c1-2-3-4-7-14-29-21(24)19-8-5-6-9-20(19)22(25)30-16-15-28-18-
InchiKey: CXNNGUNRENCHQQ-UHFFFAOYSA-N
Formula: C22H25NO7
SMILES: CCCCCCOC(=O)c1ccccc1C(=O)OCCOc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 415.44

Physical Properties

Property code	Value	Unit	Source
gf	-197.37	kJ/mol	Joback Method
hf	-679.87	kJ/mol	Joback Method
hfus	58.16	kJ/mol	Joback Method
hvap	107.76	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	4.568		Crippen Method
mcvol	311.490	ml/mol	McGowan Method
pc	1466.85	kPa	Joback Method
rinpol	3636.00		NIST Webbook
rinpol	3636.00		NIST Webbook
tb	1092.92	K	Joback Method
tc	1341.10	K	Joback Method
tf	725.74	K	Joback Method
vc	1.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1016.05	J/mol×K	1092.92	Joback Method
cpg	1024.31	J/mol×K	1134.28	Joback Method
cpg	1030.85	J/mol×K	1175.65	Joback Method
cpg	1035.69	J/mol×K	1217.01	Joback Method
cpg	1038.88	J/mol×K	1258.38	Joback Method
cpg	1040.44	J/mol×K	1299.74	Joback Method
cpg	1040.43	J/mol×K	1341.10	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=U382576&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