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

Inchi: InChI=1S/C24H29NO7/c1-2-3-4-5-6-9-16-31-23(26)21-10-7-8-11-22(21)24(27)32-18-17-
InchiKey: HXDGHFFSWHYOMD-UHFFFAOYSA-N
Formula: C24H29NO7
SMILES: CCCCCCCCOC(=O)c1ccccc1C(=O)OCCOc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 443.49

Physical Properties

Property code	Value	Unit	Source
gf	-180.53	kJ/mol	Joback Method
hf	-721.15	kJ/mol	Joback Method
hfus	63.34	kJ/mol	Joback Method
hvap	112.21	kJ/mol	Joback Method
log10ws	-7.31		Crippen Method
logp	5.348		Crippen Method
mcvol	339.670	ml/mol	McGowan Method
pc	1272.78	kPa	Joback Method
rinpol	3838.00		NIST Webbook
rinpol	3838.00		NIST Webbook
tb	1138.68	K	Joback Method
tc	1394.11	K	Joback Method
tf	748.28	K	Joback Method
vc	1.312	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1133.69	J/mol×K	1138.68	Joback Method
cpg	1141.64	J/mol×K	1181.25	Joback Method
cpg	1147.71	J/mol×K	1223.82	Joback Method
cpg	1151.95	J/mol×K	1266.40	Joback Method
cpg	1154.42	J/mol×K	1308.97	Joback Method
cpg	1155.17	J/mol×K	1351.54	Joback Method
cpg	1154.25	J/mol×K	1394.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382578&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

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