Phthalic acid, 2-(2-nitrophenyl)ethyl octyl ester

Inchi: InChI=1S/C24H29NO6/c1-2-3-4-5-6-11-17-30-23(26)20-13-8-9-14-21(20)24(27)31-18-16
InchiKey: BLMDZKJOWYNUFM-UHFFFAOYSA-N
Formula: C24H29NO6
SMILES: CCCCCCCCOC(=O)c1ccccc1C(=O)OCCc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 427.49

Physical Properties

Property code	Value	Unit	Source
gf	-75.53	kJ/mol	Joback Method
hf	-588.93	kJ/mol	Joback Method
hfus	62.15	kJ/mol	Joback Method
hvap	109.80	kJ/mol	Joback Method
log10ws	-7.57		Crippen Method
logp	5.512		Crippen Method
mcvol	333.800	ml/mol	McGowan Method
pc	1288.36	kPa	Joback Method
rinpol	3245.00		NIST Webbook
tb	1116.26	K	Joback Method
tc	1367.44	K	Joback Method
tf	726.05	K	Joback Method
vc	1.294	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1111.69	J/mol×K	1116.26	Joback Method
cpg	1121.49	J/mol×K	1158.12	Joback Method
cpg	1129.73	J/mol×K	1199.99	Joback Method
cpg	1136.48	J/mol×K	1241.85	Joback Method
cpg	1141.80	J/mol×K	1283.71	Joback Method
cpg	1145.79	J/mol×K	1325.58	Joback Method
cpg	1148.51	J/mol×K	1367.44	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=U377998&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