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

Inchi: InChI=1S/C21H23NO6/c1-2-3-8-14-27-20(23)17-10-5-6-11-18(17)21(24)28-15-13-16-9-4

InchiKey: KQLSKKQGAUFZFS-UHFFFAOYSA-N

Formula: C21H23NO6

SMILES: CCCCCOC(=O)c1ccccc1C(=O)OCCc1ccccc1[N+](=O)[O-]

Mol. weight [g/mol]: 385.41

Physical Properties

Property code	Value	Unit	Source
gf	-100.79	kJ/mol	Joback Method
hf	-527.01	kJ/mol	Joback Method
hfus	54.38	kJ/mol	Joback Method
hvap	103.12	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	4.341		Crippen Method
mcvol	291.530	ml/mol	McGowan Method
pc	1602.56	kPa	Joback Method
rinpol	2940.00		NIST Webbook
rinpol	2940.00		NIST Webbook
tb	1047.62	K	Joback Method
tc	1292.43	K	Joback Method
tf	692.24	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	934.26	J/mol×K	1047.62	Joback Method
cpg	944.10	J/mol×K	1088.42	Joback Method
cpg	952.50	J/mol×K	1129.22	Joback Method
cpg	959.49	J/mol×K	1170.03	Joback Method
cpg	965.15	J/mol×K	1210.83	Joback Method
cpg	969.52	J/mol×K	1251.63	Joback Method
cpg	972.66	J/mol×K	1292.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377995&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