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

Inchi: InChI=1S/C23H27NO6/c1-2-3-4-5-10-16-29-22(25)19-12-7-8-13-20(19)23(26)30-17-15-1

InchiKey: ORMVQFLBOKRHIW-UHFFFAOYSA-N

Formula: C23H27NO6

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

Mol. weight [g/mol]: 413.46

Physical Properties

Property code	Value	Unit	Source
gf	-83.95	kJ/mol	Joback Method
hf	-568.29	kJ/mol	Joback Method
hfus	59.56	kJ/mol	Joback Method
hvap	107.57	kJ/mol	Joback Method
log10ws	-7.15		Crippen Method
logp	5.121		Crippen Method
mcvol	319.710	ml/mol	McGowan Method
pc	1381.96	kPa	Joback Method
rinpol	3142.00		NIST Webbook
tb	1093.38	K	Joback Method
tc	1341.38	K	Joback Method
tf	714.78	K	Joback Method
vc	1.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1052.16	J/mol×K	1093.38	Joback Method
cpg	1061.98	J/mol×K	1134.71	Joback Method
cpg	1070.28	J/mol×K	1176.05	Joback Method
cpg	1077.12	J/mol×K	1217.38	Joback Method
cpg	1082.58	J/mol×K	1258.71	Joback Method
cpg	1086.72	J/mol×K	1300.04	Joback Method
cpg	1089.60	J/mol×K	1341.38	Joback Method

Sources

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=U377997&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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