

# Phthalic acid, heptyl 2-(4-nitrophenoxy)ethyl ester

Inchi:	InChI=1S/C23H27NO7/c1-2-3-4-5-8-15-30-22(25)20-9-6-7-10-21(20)23(26)31-17-16-29-
InchiKey:	WHGFDFCNXFPWQI-UHFFFAOYSA-N
Formula:	C23H27NO7
SMILES:	CCCCCCCOC(=O)c1ccccc1C(=O)OCCOc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	429.46

## Physical Properties

Property code	Value	Unit	Source
gf	-188.95	kJ/mol	Joback Method
hf	-700.51	kJ/mol	Joback Method
hfus	60.75	kJ/mol	Joback Method
hvap	109.98	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	4.958		Crippen Method
mcvol	325.580	ml/mol	McGowan Method
pc	1364.66	kPa	Joback Method
rinpola	3736.00		NIST Webbook
rinpola	3736.00		NIST Webbook
tb	1115.80	K	Joback Method
tc	1367.04	K	Joback Method
tf	737.01	K	Joback Method
vc	1.256	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1074.73	J/molxK	1115.80	Joback Method
cpg	1082.85	J/molxK	1157.67	Joback Method
cpg	1089.16	J/molxK	1199.55	Joback Method
cpg	1093.72	J/molxK	1241.42	Joback Method
cpg	1096.58	J/molxK	1283.29	Joback Method
cpg	1097.76	J/molxK	1325.17	Joback Method
cpg	1097.33	J/molxK	1367.04	Joback Method

# Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U382577&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382577&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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