

# Phthalic acid, isobutyl 2-(2-nitrophenyl)ethyl ester

Inchi:	InChI=1S/C20H21NO6/c1-14(2)13-27-20(23)17-9-5-4-8-16(17)19(22)26-12-11-15-7-3-6-
InchiKey:	QTVDSHLPBUGLFZ-UHFFFAOYSA-N
Formula:	C20H21NO6
SMILES:	CC(C)COC(=O)c1ccccc1C(=O)OCCc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	371.38

## Physical Properties

Property code	Value	Unit	Source
gf	-111.65	kJ/mol	Joback Method
hf	-511.65	kJ/mol	Joback Method
hfus	48.27	kJ/mol	Joback Method
hvap	100.51	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	3.807		Crippen Method
mcvol	277.440	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
rinqol	2797.00		NIST Webbook
tb	1024.30	K	Joback Method
tc	1271.22	K	Joback Method
tf	665.97	K	Joback Method
vc	1.063	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	876.34	J/molxK	1024.30	Joback Method
cpg	886.19	J/molxK	1065.45	Joback Method
cpg	894.56	J/molxK	1106.61	Joback Method
cpg	901.53	J/molxK	1147.76	Joback Method
cpg	907.13	J/molxK	1188.91	Joback Method
cpg	911.41	J/molxK	1230.07	Joback Method
cpg	914.43	J/molxK	1271.22	Joback Method

# Sources

<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>
<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=U377993&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377993&amp;Units=SI</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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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