

# Phthalic acid, heptyl 3-methoxybenzyl ester

<b>Inchi:</b>	InChI=1S/C23H28O5/c1-3-4-5-6-9-15-27-22(24)20-13-7-8-14-21(20)23(25)28-17-18-11-
<b>InchiKey:</b>	XXSXNUSHWJJXEH-UHFFFAOYSA-N
<b>Formula:</b>	C23H28O5
<b>SMILES:</b>	CCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccc(OC)c1
<b>Mol. weight [g/mol]:</b>	384.47

## Physical Properties

Property code	Value	Unit	Source
gf	-224.50	kJ/mol	Joback Method
hf	-689.75	kJ/mol	Joback Method
hfus	49.39	kJ/mol	Joback Method
hvap	93.39	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	5.179		Crippen Method
mcvol	308.160	ml/mol	McGowan Method
pc	1352.64	kPa	Joback Method
rinpol	2900.00		NIST Webbook
tb	963.96	K	Joback Method
tc	1187.86	K	Joback Method
tf	593.40	K	Joback Method
vc	1.173	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	983.39	J/molxK	963.96	Joback Method
cpg	1035.43	J/molxK	1150.55	Joback Method
cpg	1027.94	J/molxK	1113.23	Joback Method
cpg	1019.01	J/molxK	1075.91	Joback Method
cpg	1008.63	J/molxK	1038.59	Joback Method
cpg	996.76	J/molxK	1001.28	Joback Method
cpg	1041.52	J/molxK	1187.86	Joback Method
dvisc	0.0000280	Paxs	963.96	Joback Method
dvisc	0.0000353	Paxs	902.20	Joback Method

dvisc	0.0000462	Paxs	840.44	Joback Method
dvisc	0.0000631	Paxs	778.68	Joback Method
dvisc	0.0000909	Paxs	716.92	Joback Method
dvisc	0.0001403	Paxs	655.16	Joback Method
dvisc	0.0002370	Paxs	593.40	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U377980&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377980&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>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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