

# Phthalic acid, 2,4-dimethylpent-3-yl heptyl ester

Inchi:	InChI=1S/C22H34O4/c1-6-7-8-9-12-15-25-21(23)18-13-10-11-14-19(18)22(24)26-20(16)
InchiKey:	WEOFEVBZOFAIBU-UHFFFAOYSA-N
Formula:	C22H34O4
SMILES:	CCCCCCCOC(=O)c1ccccc1C(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]:	362.50

## Physical Properties

Property code	Value	Unit	Source
gf	-238.02	kJ/mol	Joback Method
hf	-777.79	kJ/mol	Joback Method
hfus	41.39	kJ/mol	Joback Method
hvap	84.65	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	5.651		Crippen Method
mvol	311.960	ml/mol	McGowan Method
pc	1190.70	kPa	Joback Method
rinpol	2396.00		NIST Webbook
rinpol	2396.00		NIST Webbook
tb	885.68	K	Joback Method
tc	1092.54	K	Joback Method
tf	475.96	K	Joback Method
vc	1.190	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.73	J/molxK	885.68	Joback Method
cpg	1015.52	J/molxK	920.16	Joback Method
cpg	1031.00	J/molxK	954.63	Joback Method
cpg	1045.19	J/molxK	989.11	Joback Method
cpg	1058.14	J/molxK	1023.59	Joback Method
cpg	1069.87	J/molxK	1058.07	Joback Method
cpg	1080.41	J/molxK	1092.54	Joback Method
dvisc	0.0007173	Paxs	475.96	Joback Method

dvisc	0.0003074	Paxs	544.25	Joback Method
dvisc	0.0001592	Paxs	612.53	Joback Method
dvisc	0.0000940	Paxs	680.82	Joback Method
dvisc	0.0000611	Paxs	749.11	Joback Method
dvisc	0.0000427	Paxs	817.39	Joback Method
dvisc	0.0000315	Paxs	885.68	Joback Method

## Sources

<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=U356846&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356846&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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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