

# Phthalic acid, decyl 2,4,4-trimethylpentyl ester

<b>Inchi:</b>	InChI=1S/C26H42O4/c1-6-7-8-9-10-11-12-15-18-29-24(27)22-16-13-14-17-23(22)25(28)
<b>InchiKey:</b>	GXMJDROWJFZMDM-UHFFFAOYSA-N
<b>Formula:</b>	C26H42O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)c1ccccc1C(=O)OCC(C)CC(C)(C)C
<b>Mol. weight [g/mol]:</b>	418.61

## Physical Properties

Property code	Value	Unit	Source
gf	-196.62	kJ/mol	Joback Method
hf	-858.54	kJ/mol	Joback Method
hfus	51.38	kJ/mol	Joback Method
hvap	93.04	kJ/mol	Joback Method
log10ws	-8.17		Crippen Method
logp	7.213		Crippen Method
mcvol	368.320	ml/mol	McGowan Method
pc	930.07	kPa	Joback Method
rinsol	2786.00		NIST Webbook
tb	974.85	K	Joback Method
tc	1193.64	K	Joback Method
tf	553.46	K	Joback Method
vc	1.415	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1243.96	J/molxK	974.85	Joback Method
cpg	1261.44	J/molxK	1011.31	Joback Method
cpg	1277.49	J/molxK	1047.78	Joback Method
cpg	1292.20	J/molxK	1084.24	Joback Method
cpg	1305.62	J/molxK	1120.71	Joback Method
cpg	1317.83	J/molxK	1157.17	Joback Method
cpg	1328.91	J/molxK	1193.64	Joback Method
dvisc	0.0002960	Paxs	553.46	Joback Method
dvisc	0.0001378	Paxs	623.69	Joback Method

dvisc	0.0000749	Paxs	693.92	Joback Method
dvisc	0.0000456	Paxs	764.15	Joback Method
dvisc	0.0000301	Paxs	834.39	Joback Method
dvisc	0.0000212	Paxs	904.62	Joback Method
dvisc	0.0000158	Paxs	974.85	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=U377776&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377776&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>

## 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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