

# Trimellitic acid, 2,2,4-trimethylpentyl ester

<b>Inchi:</b>	InChI=1S/C33H54O6/c1-22(2)16-31(7,8)19-37-28(34)25-13-14-26(29(35)38-20-32(9,10)
<b>InchiKey:</b>	GFNQLDIWJXUYKC-UHFFFAOYSA-N
<b>Formula:</b>	C33H54O6
<b>SMILES:</b>	CC(C)CC(C)(C)COC(=O)c1ccc(C(=O)OCC(C)(C)CC(C)C)c(C(=O)OCC(C)(C)CC(C)C)c1
<b>Mol. weight [g/mol]:</b>	546.78
<b>CAS:</b>	53046-84-7

## Physical Properties

Property code	Value	Unit	Source
gf	-380.43	kJ/mol	Joback Method
hf	-1287.35	kJ/mol	Joback Method
hfus	50.04	kJ/mol	Joback Method
hvap	115.07	kJ/mol	Joback Method
log10ws	-9.54		Crippen Method
logp	8.374		Crippen Method
mcvol	474.390	ml/mol	McGowan Method
pc	669.08	kPa	Joback Method
tb	1208.94	K	Joback Method
tc	1498.91	K	Joback Method
tf	691.87	K	Joback Method
vc	1.796	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1724.23	J/molxK	1208.94	Joback Method
cpg	1740.94	J/molxK	1257.27	Joback Method
cpg	1755.91	J/molxK	1305.60	Joback Method
cpg	1769.40	J/molxK	1353.93	Joback Method
cpg	1781.67	J/molxK	1402.26	Joback Method
cpg	1792.97	J/molxK	1450.58	Joback Method
cpg	1803.57	J/molxK	1498.91	Joback Method
dvisc	0.0000382	Paxs	691.87	Joback Method
dvisc	0.0000164	Paxs	778.05	Joback Method

dvisc	0.0000083	Paxs	864.23	Joback Method
dvisc	0.0000048	Paxs	950.40	Joback Method
dvisc	0.0000030	Paxs	1036.58	Joback Method
dvisc	0.0000020	Paxs	1122.76	Joback Method
dvisc	0.0000015	Paxs	1208.94	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C53046847&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C53046847&amp;Units=SI</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>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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