

# Terephthalic acid, dodec-2-enyl heptyl ester

<b>Inchi:</b>	InChI=1S/C27H42O4/c1-3-5-7-9-10-11-12-13-15-17-23-31-27(29)25-20-18-24(19-21-25)
<b>InchiKey:</b>	VAXFBHMLDMPZTE-BMRADRMJSA-N
<b>Formula:</b>	C27H42O4
<b>SMILES:</b>	CCCCCCCCC=CCOC(=O)c1ccc(C(=O)OCCCCCCC)cc1
<b>Mol. weight [g/mol]:</b>	430.62

## Physical Properties

Property code	Value	Unit	Source
gf	-108.38	kJ/mol	Joback Method
hf	-747.93	kJ/mol	Joback Method
hfus	65.11	kJ/mol	Joback Method
hvap	96.90	kJ/mol	Joback Method
log10ws	-8.93		Crippen Method
logp	7.668		Crippen Method
mcvol	378.110	ml/mol	McGowan Method
pc	891.07	kPa	Joback Method
rinpola	3332.00		NIST Webbook
tb	1005.56	K	Joback Method
tc	1232.11	K	Joback Method
tf	572.23	K	Joback Method
vc	1.468	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1277.89	J/molxK	1005.56	Joback Method
cpg	1295.50	J/molxK	1043.32	Joback Method
cpg	1311.64	J/molxK	1081.08	Joback Method
cpg	1326.39	J/molxK	1118.83	Joback Method
cpg	1339.83	J/molxK	1156.59	Joback Method
cpg	1352.04	J/molxK	1194.35	Joback Method
cpg	1363.08	J/molxK	1232.11	Joback Method
dvisc	0.0002485	Paxs	572.23	Joback Method
dvisc	0.0001241	Paxs	644.45	Joback Method

dvisc	0.0000712	Paxs	716.67	Joback Method
dvisc	0.0000453	Paxs	788.89	Joback Method
dvisc	0.0000311	Paxs	861.12	Joback Method
dvisc	0.0000226	Paxs	933.34	Joback Method
dvisc	0.0000172	Paxs	1005.56	Joback Method

## Sources

<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=U356308&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356308&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>

## 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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