

# Terephthalic acid, dodec-2-enyl isobutyl ester

<b>Inchi:</b>	InChI=1S/C24H36O4/c1-4-5-6-7-8-9-10-11-12-13-18-27-23(25)21-14-16-22(17-15-21)24
<b>InchiKey:</b>	MVZGITWJZFKYFS-OUKQBFOZSA-N
<b>Formula:</b>	C24H36O4
<b>SMILES:</b>	CCCCCCCCC=CCOC(=O)c1ccc(C(=O)OCC(C)C)cc1
<b>Mol. weight [g/mol]:</b>	388.54

## Physical Properties

Property code	Value	Unit	Source
gf	-136.08	kJ/mol	Joback Method
hf	-691.29	kJ/mol	Joback Method
hfus	53.82	kJ/mol	Joback Method
hvap	89.84	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	6.353		Crippen Method
mvol	335.840	ml/mol	McGowan Method
pc	1072.17	kPa	Joback Method
rinpol	2938.00		NIST Webbook
rinpol	2938.00		NIST Webbook
tb	936.48	K	Joback Method
tc	1148.54	K	Joback Method
tf	523.42	K	Joback Method
vc	1.294	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1091.95	J/molxK	936.48	Joback Method
cpg	1108.59	J/molxK	971.82	Joback Method
cpg	1123.96	J/molxK	1007.17	Joback Method
cpg	1138.11	J/molxK	1042.51	Joback Method
cpg	1151.11	J/molxK	1077.86	Joback Method
cpg	1162.98	J/molxK	1113.20	Joback Method
cpg	1173.80	J/molxK	1148.54	Joback Method
dvisc	0.0003980	Paxs	523.42	Joback Method

dvisc	0.0001911	Paxs	592.26	Joback Method
dvisc	0.0001069	Paxs	661.11	Joback Method
dvisc	0.0000668	Paxs	729.95	Joback Method
dvisc	0.0000452	Paxs	798.79	Joback Method
dvisc	0.0000326	Paxs	867.64	Joback Method
dvisc	0.0000246	Paxs	936.48	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=U356303&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356303&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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