

# Dimethylmalonic acid, dodecyl 2-isopropoxyphenyl ester

**Inchi:** InChI=1S/C26H42O5/c1-6-7-8-9-10-11-12-13-14-17-20-29-24(27)26(4,5)25(28)31-23-19  
**InchiKey:** YIEZQINOCYMDQ-UHFFFAOYSA-N  
**Formula:** C26H42O5  
**SMILES:** CCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1ccccc1OC(C)C  
**Mol. weight [g/mol]:** 434.61

## Physical Properties

Property code	Value	Unit	Source
gf	-301.62	kJ/mol	Joback Method
hf	-990.76	kJ/mol	Joback Method
hfus	52.57	kJ/mol	Joback Method
hvap	95.45	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	6.870		Crippen Method
mvol	374.190	ml/mol	McGowan Method
pc	920.50	kPa	Joback Method
rinpol	2749.00		NIST Webbook
rinpol	2749.00		NIST Webbook
tb	997.27	K	Joback Method
tc	1221.01	K	Joback Method
tf	575.69	K	Joback Method
vc	1.433	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1273.39	J/molxK	997.27	Joback Method
cpg	1341.33	J/molxK	1183.72	Joback Method
cpg	1330.72	J/molxK	1146.43	Joback Method
cpg	1318.68	J/molxK	1109.14	Joback Method
cpg	1305.15	J/molxK	1071.85	Joback Method
cpg	1290.07	J/molxK	1034.56	Joback Method
cpg	1350.57	J/molxK	1221.01	Joback Method
dvisc	0.0000115	Paxs	997.27	Joback Method

dvisc	0.0000155	Paxs	927.01	Joback Method
dvisc	0.0000218	Paxs	856.74	Joback Method
dvisc	0.0000327	Paxs	786.48	Joback Method
dvisc	0.0000530	Paxs	716.22	Joback Method
dvisc	0.0000955	Paxs	645.95	Joback Method
dvisc	0.0001987	Paxs	575.69	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=U361860&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361860&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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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