

# Dimethylmalonic acid, 3-phenylpropyl undecyl ester

Inchi:	InChI=1S/C25H40O4/c1-4-5-6-7-8-9-10-11-15-20-28-23(26)25(2,3)24(27)29-21-16-19-22
InchiKey:	LIWDTDKVKYHISX-UHFFFAOYSA-N
Formula:	C25H40O4
SMILES:	CCCCCCCCCOC(=O)C(C)(C)C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	404.58

## Physical Properties

Property code	Value	Unit	Source
gf	-192.97	kJ/mol	Joback Method
hf	-821.15	kJ/mol	Joback Method
hfus	52.71	kJ/mol	Joback Method
hvap	90.54	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	6.263		Crippen Method
mcvol	354.230	ml/mol	McGowan Method
pc	991.38	kPa	Joback Method
rinsol	2726.00		NIST Webbook
tb	947.43	K	Joback Method
tc	1160.67	K	Joback Method
tf	544.67	K	Joback Method
vc	1.365	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1181.88	J/molxK	947.43	Joback Method
cpg	1256.11	J/molxK	1125.13	Joback Method
cpg	1243.64	J/molxK	1089.59	Joback Method
cpg	1230.05	J/molxK	1054.05	Joback Method
cpg	1215.27	J/molxK	1018.51	Joback Method
cpg	1199.24	J/molxK	982.97	Joback Method
cpg	1267.53	J/molxK	1160.67	Joback Method
dvisc	0.0000199	Paxs	947.43	Joback Method
dvisc	0.0000267	Paxs	880.30	Joback Method

dvisc	0.0000377	Paxs	813.18	Joback Method
dvisc	0.0000566	Paxs	746.05	Joback Method
dvisc	0.0000920	Paxs	678.92	Joback Method
dvisc	0.0001667	Paxs	611.80	Joback Method
dvisc	0.0003495	Paxs	544.67	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=U361840&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361840&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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