

# Dimethylmalonic acid, 3-methylphenyl octyl ester

Inchi:	InChI=1S/C20H30O4/c1-5-6-7-8-9-10-14-23-18(21)20(3,4)19(22)24-17-13-11-12-16(2)15
InchiKey:	ILLDYJQRTVUYBY-UHFFFAOYSA-N
Formula:	C20H30O4
SMILES:	CCCCCCCCOC(=O)C(C)(C)C(=O)Oc1cccc(C)c1
Mol. weight [g/mol]:	334.45

## Physical Properties

Property code	Value	Unit	Source
gf	-244.70	kJ/mol	Joback Method
hf	-729.42	kJ/mol	Joback Method
hfus	39.37	kJ/mol	Joback Method
hvap	80.07	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	4.830		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1360.63	kPa	Joback Method
rinpol	2193.00		NIST Webbook
tb	838.01	K	Joback Method
tc	1043.17	K	Joback Method
tf	500.84	K	Joback Method
vc	1.085	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.75	J/molxK	838.01	Joback Method
cpg	895.04	J/molxK	872.20	Joback Method
cpg	910.18	J/molxK	906.40	Joback Method
cpg	924.22	J/molxK	940.59	Joback Method
cpg	937.18	J/molxK	974.79	Joback Method
cpg	949.13	J/molxK	1008.98	Joback Method
cpg	960.08	J/molxK	1043.17	Joback Method
dvisc	0.0005463	Paxs	500.84	Joback Method
dvisc	0.0002895	Paxs	557.03	Joback Method

dvisc	0.0001723	Paxs	613.23	Joback Method
dvisc	0.0001119	Paxs	669.42	Joback Method
dvisc	0.0000777	Paxs	725.62	Joback Method
dvisc	0.0000569	Paxs	781.82	Joback Method
dvisc	0.0000434	Paxs	838.01	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=U363616&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U363616&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

Latest version available from:

<https://www.chemeo.com/cid/65-470-8/Dimethylmalonic-acid-3-methylphenyl-octyl-ester.pdf>

Generated by Cheméo on 2024-04-29 15:38:37.954671515 +0000 UTC m=+16694366.875248837.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.