

# Diethylmalonic acid, 2-isopropylphenyl octyl ester

Inchi:	InChI=1S/C24H38O4/c1-6-9-10-11-12-15-18-27-22(25)24(7-2,8-3)23(26)28-21-17-14-13
InchiKey:	OYWLAYRVWXUMBG-UHFFFAOYSA-N
Formula:	C24H38O4
SMILES:	CCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1C(C)C
Mol. weight [g/mol]:	390.56

## Physical Properties

Property code	Value	Unit	Source
gf	-213.46	kJ/mol	Joback Method
hf	-817.26	kJ/mol	Joback Method
hfus	46.20	kJ/mol	Joback Method
hvap	88.58	kJ/mol	Joback Method
log10ws	-7.03		Crippen Method
logp	6.425		Crippen Method
mcvol	340.140	ml/mol	McGowan Method
pc	1049.37	kPa	Joback Method
rinqol	2417.00		NIST Webbook
tb	929.09	K	Joback Method
tc	1140.66	K	Joback Method
tf	530.92	K	Joback Method
vc	1.302	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1120.03	J/molxK	929.09	Joback Method
cpg	1137.08	J/molxK	964.35	Joback Method
cpg	1152.82	J/molxK	999.61	Joback Method
cpg	1167.30	J/molxK	1034.87	Joback Method
cpg	1180.59	J/molxK	1070.14	Joback Method
cpg	1192.72	J/molxK	1105.40	Joback Method
cpg	1203.78	J/molxK	1140.66	Joback Method
dvisc	0.0003846	Paxs	530.92	Joback Method
dvisc	0.0001823	Paxs	597.28	Joback Method

dvisc	0.0001003	Paxs	663.64	Joback Method
dvisc	0.0000616	Paxs	730.00	Joback Method
dvisc	0.0000410	Paxs	796.37	Joback Method
dvisc	0.0000290	Paxs	862.73	Joback Method
dvisc	0.0000216	Paxs	929.09	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=U369973&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369973&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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