

# Diethylmalonic acid, dodecyl 5-methoxy-3-methylpentyl ester

<b>Inchi:</b>	InChI=1S/C26H50O5/c1-6-9-10-11-12-13-14-15-16-17-20-30-24(27)26(7-2,8-3)25(28)31
<b>InchiKey:</b>	BHRYEPQCALICHN-UHFFFAOYSA-N
<b>Formula:</b>	C26H50O5
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCC(C)CCOC
<b>Mol. weight [g/mol]:</b>	442.67

## Physical Properties

Property code	Value	Unit	Source
gf	-404.40	kJ/mol	Joback Method
hf	-1215.82	kJ/mol	Joback Method
hfus	58.92	kJ/mol	Joback Method
hvap	92.51	kJ/mol	Joback Method
log10ws	-7.03		Crippen Method
logp	6.863		Crippen Method
mcvol	397.950	ml/mol	McGowan Method
pc	766.49	kPa	Joback Method
rinpol	2700.00		NIST Webbook
tb	965.61	K	Joback Method
tc	1187.20	K	Joback Method
tf	536.75	K	Joback Method
vc	1.540	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1377.22	J/molxK	965.61	Joback Method
cpg	1397.58	J/molxK	1002.54	Joback Method
cpg	1416.22	J/molxK	1039.47	Joback Method
cpg	1433.19	J/molxK	1076.41	Joback Method
cpg	1448.55	J/molxK	1113.34	Joback Method
cpg	1462.35	J/molxK	1150.27	Joback Method
cpg	1474.65	J/molxK	1187.20	Joback Method
dvisc	0.0002765	Paxs	536.75	Joback Method
dvisc	0.0001178	Paxs	608.23	Joback Method

dvisc	0.0000601	Paxs	679.70	Joback Method
dvisc	0.0000348	Paxs	751.18	Joback Method
dvisc	0.0000222	Paxs	822.66	Joback Method
dvisc	0.0000152	Paxs	894.13	Joback Method
dvisc	0.0000110	Paxs	965.61	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U370771&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370771&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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