

# Diethylmalonic acid, decyl nonyl ester

<b>Inchi:</b>	InChI=1S/C26H50O4/c1-5-9-11-13-15-17-19-21-23-30-25(28)26(7-3,8-4)24(27)29-22-20
<b>InchiKey:</b>	ZQUUKHBZDJEHHE-UHFFFAOYSA-N
<b>Formula:</b>	C26H50O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCCCCCC
<b>Mol. weight [g/mol]:</b>	426.67

## Physical Properties

Property code	Value	Unit	Source
gf	-296.96	kJ/mol	Joback Method
hf	-1078.32	kJ/mol	Joback Method
hfus	61.26	kJ/mol	Joback Method
hvap	90.49	kJ/mol	Joback Method
log10ws	-8.19		Crippen Method
logp	7.771		Crippen Method
mcvol	392.080	ml/mol	McGowan Method
pc	770.32	kPa	Joback Method
rinpol	2750.00		NIST Webbook
tb	943.63	K	Joback Method
tc	1158.72	K	Joback Method
tf	529.52	K	Joback Method
vc	1.528	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1344.97	J/molxK	943.63	Joback Method
cpg	1365.90	J/molxK	979.48	Joback Method
cpg	1385.32	J/molxK	1015.33	Joback Method
cpg	1403.28	J/molxK	1051.17	Joback Method
cpg	1419.86	J/molxK	1087.02	Joback Method
cpg	1435.13	J/molxK	1122.87	Joback Method
cpg	1449.14	J/molxK	1158.72	Joback Method
dvisc	0.0003659	Paxs	529.52	Joback Method
dvisc	0.0001622	Paxs	598.54	Joback Method

dvisc	0.0000851	Paxs	667.56	Joback Method
dvisc	0.0000504	Paxs	736.58	Joback Method
dvisc	0.0000326	Paxs	805.59	Joback Method
dvisc	0.0000226	Paxs	874.61	Joback Method
dvisc	0.0000166	Paxs	943.63	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=U369463&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369463&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

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