

# Diethylmalonic acid, heptyl undecyl ester

<b>Inchi:</b>	InChI=1S/C25H48O4/c1-5-9-11-13-14-15-16-18-20-22-29-24(27)25(7-3,8-4)23(26)28-21
<b>InchiKey:</b>	WDTQZPHLRWWMFJ-UHFFFAOYSA-N
<b>Formula:</b>	C25H48O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCCCC
<b>Mol. weight [g/mol]:</b>	412.65

## Physical Properties

Property code	Value	Unit	Source
gf	-305.38	kJ/mol	Joback Method
hf	-1057.68	kJ/mol	Joback Method
hfus	58.67	kJ/mol	Joback Method
hvap	88.26	kJ/mol	Joback Method
log10ws	-7.77		Crippen Method
logp	7.380		Crippen Method
mcvol	377.990	ml/mol	McGowan Method
pc	813.07	kPa	Joback Method
rinsol	2556.00		NIST Webbook
tb	920.75	K	Joback Method
tc	1128.53	K	Joback Method
tf	518.25	K	Joback Method
vc	1.472	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1281.05	J/molxK	920.75	Joback Method
cpg	1369.40	J/molxK	1093.90	Joback Method
cpg	1354.32	J/molxK	1059.27	Joback Method
cpg	1338.00	J/molxK	1024.64	Joback Method
cpg	1320.39	J/molxK	990.01	Joback Method
cpg	1301.43	J/molxK	955.38	Joback Method
cpg	1383.30	J/molxK	1128.53	Joback Method
dvisc	0.0000195	Paxs	920.75	Joback Method
dvisc	0.0000265	Paxs	853.67	Joback Method

dvisc	0.0000382	Paxs	786.58	Joback Method
dvisc	0.0000588	Paxs	719.50	Joback Method
dvisc	0.0000990	Paxs	652.42	Joback Method
dvisc	0.0001876	Paxs	585.33	Joback Method
dvisc	0.0004198	Paxs	518.25	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U369519&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369519&amp;Units=SI</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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