

# Diethylmalonic acid, decyl 2,4,4-trimethylpentyl ester

Inchi:	InChI=1S/C25H48O4/c1-8-11-12-13-14-15-16-17-18-28-22(26)25(9-2,10-3)23(27)29-20-
InchiKey:	LHASJMFCRWBEQB-UHFFFAOYSA-N
Formula:	C25H48O4
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	412.65

## Physical Properties

Property code	Value	Unit	Source
gf	-304.98	kJ/mol	Joback Method
hf	-1071.71	kJ/mol	Joback Method
hfus	47.73	kJ/mol	Joback Method
hvap	86.58	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	7.092		Crippen Method
mcvol	377.990	ml/mol	McGowan Method
pc	825.74	kPa	Joback Method
rinpol	2413.00		NIST Webbook
tb	917.08	K	Joback Method
tc	1122.77	K	Joback Method
tf	505.67	K	Joback Method
vc	1.456	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1281.38	J/molxK	917.08	Joback Method
cpg	1301.42	J/molxK	951.36	Joback Method
cpg	1320.15	J/molxK	985.64	Joback Method
cpg	1337.62	J/molxK	1019.92	Joback Method
cpg	1353.92	J/molxK	1054.20	Joback Method
cpg	1369.12	J/molxK	1088.48	Joback Method
cpg	1383.30	J/molxK	1122.77	Joback Method
dvisc	0.0004445	Paxs	505.67	Joback Method
dvisc	0.0001762	Paxs	574.24	Joback Method

dvisc	0.0000850	Paxs	642.81	Joback Method
dvisc	0.0000472	Paxs	711.38	Joback Method
dvisc	0.0000291	Paxs	779.94	Joback Method
dvisc	0.0000194	Paxs	848.51	Joback Method
dvisc	0.0000137	Paxs	917.08	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=U369482&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369482&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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