

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

Inchi:	InChI=1S/C18H34O4/c1-8-11-21-15(19)18(9-2,10-3)16(20)22-13-14(4)12-17(5,6)7/h14H
InchiKey:	IGIBEXZUGFBEPS-UHFFFAOYSA-N
Formula:	C18H34O4
SMILES:	CCCOC(=O)C(CC)(CC)C(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	314.46

## Physical Properties

Property code	Value	Unit	Source
gf	-363.92	kJ/mol	Joback Method
hf	-927.23	kJ/mol	Joback Method
hfus	29.60	kJ/mol	Joback Method
hvap	70.99	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.362		Crippen Method
mvol	279.360	ml/mol	McGowan Method
pc	1268.25	kPa	Joback Method
rinpol	1746.00		NIST Webbook
rinpol	1746.00		NIST Webbook
tb	756.92	K	Joback Method
tc	946.57	K	Joback Method
tf	426.78	K	Joback Method
vc	1.063	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.13	J/molxK	756.92	Joback Method
cpg	871.12	J/molxK	788.53	Joback Method
cpg	888.06	J/molxK	820.14	Joback Method
cpg	903.99	J/molxK	851.74	Joback Method
cpg	918.95	J/molxK	883.35	Joback Method
cpg	932.99	J/molxK	914.96	Joback Method
cpg	946.14	J/molxK	946.57	Joback Method
dvisc	0.0012202	Paxs	426.78	Joback Method

dvisc	0.0005099	Paxs	481.80	Joback Method
dvisc	0.0002548	Paxs	536.83	Joback Method
dvisc	0.0001449	Paxs	591.85	Joback Method
dvisc	0.0000907	Paxs	646.87	Joback Method
dvisc	0.0000611	Paxs	701.90	Joback Method
dvisc	0.0000436	Paxs	756.92	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=U369474&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369474&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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