

# Diethylmalonic acid, 3-methylpent-2-yl propyl ester

Inchi:	InChI=1S/C16H30O4/c1-7-11-19-14(17)16(9-3,10-4)15(18)20-13(6)12(5)8-2/h12-13H,7-
InchiKey:	AGQUNFDBUDRDHC-UHFFFAOYSA-N
Formula:	C16H30O4
SMILES:	CCCOC(=O)C(CC)(CC)C(=O)OC(C)C(C)CC
Mol. weight [g/mol]:	286.41

## Physical Properties

Property code	Value	Unit	Source
gf	-386.04	kJ/mol	Joback Method
hf	-882.48	kJ/mol	Joback Method
hfus	28.31	kJ/mol	Joback Method
hvap	67.45	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.724		Crippen Method
mcvol	251.180	ml/mol	McGowan Method
pc	1449.04	kPa	Joback Method
rinsol	1603.00		NIST Webbook
tb	713.95	K	Joback Method
tc	900.32	K	Joback Method
tf	386.82	K	Joback Method
vc	0.957	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.65	J/molxK	713.95	Joback Method
cpg	753.98	J/molxK	745.01	Joback Method
cpg	770.36	J/molxK	776.07	Joback Method
cpg	785.81	J/molxK	807.13	Joback Method
cpg	800.36	J/molxK	838.20	Joback Method
cpg	814.03	J/molxK	869.26	Joback Method
cpg	826.83	J/molxK	900.32	Joback Method
dvisc	0.0019778	Paxs	386.82	Joback Method
dvisc	0.0007910	Paxs	441.34	Joback Method

dvisc	0.0003870	Paxs	495.86	Joback Method
dvisc	0.0002181	Paxs	550.38	Joback Method
dvisc	0.0001363	Paxs	604.91	Joback Method
dvisc	0.0000921	Paxs	659.43	Joback Method
dvisc	0.0000661	Paxs	713.95	Joback Method

## Sources

<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=U369727&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369727&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>

## 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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