

# Diethylmalonic acid, hexadecyl 3-phenylpropyl ester

Inchi:	InChI=1S/C32H54O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-22-27-35-30(33)32(5-2,6-3
InchiKey:	CGDGIEZFTQWIEH-UHFFFAOYSA-N
Formula:	C32H54O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	502.77

## Physical Properties

Property code	Value	Unit	Source
gf	-134.03	kJ/mol	Joback Method
hf	-965.63	kJ/mol	Joback Method
hfus	70.84	kJ/mol	Joback Method
hvap	106.12	kJ/mol	Joback Method
log10ws	-9.80		Crippen Method
logp	8.993		Crippen Method
mcvol	452.860	ml/mol	McGowan Method
pc	675.35	kPa	Joback Method
rinsol	3408.00		NIST Webbook
tb	1107.59	K	Joback Method
tc	1376.17	K	Joback Method
tf	623.56	K	Joback Method
vc	1.756	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1626.31	J/molxK	1107.59	Joback Method
cpg	1646.70	J/molxK	1152.35	Joback Method
cpg	1665.13	J/molxK	1197.12	Joback Method
cpg	1681.79	J/molxK	1241.88	Joback Method
cpg	1696.86	J/molxK	1286.64	Joback Method
cpg	1710.53	J/molxK	1331.40	Joback Method
cpg	1722.97	J/molxK	1376.17	Joback Method
dvisc	0.0001322	Paxs	623.56	Joback Method
dvisc	0.0000596	Paxs	704.23	Joback Method

dvisc	0.0000317	Paxs	784.90	Joback Method
dvisc	0.0000189	Paxs	865.57	Joback Method
dvisc	0.0000124	Paxs	946.25	Joback Method
dvisc	0.0000086	Paxs	1026.92	Joback Method
dvisc	0.0000063	Paxs	1107.59	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=U369666&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369666&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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