

# Diethylmalonic acid, 3-chlorobenzyl tetradecyl ester

Inchi:	InChI=1S/C28H45ClO4/c1-4-7-8-9-10-11-12-13-14-15-16-17-21-32-26(30)28(5-2,6-3)27
InchiKey:	PTBINLNVBMQKLV-UHFFFAOYSA-N
Formula:	C28H45ClO4
SMILES:	CCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1cccc(Cl)c1
Mol. weight [g/mol]:	481.11

## Physical Properties

Property code	Value	Unit	Source
gf	-189.27	kJ/mol	Joback Method
hf	-910.28	kJ/mol	Joback Method
hfus	64.28	kJ/mol	Joback Method
hvap	102.26	kJ/mol	Joback Method
log10ws	-9.31		Crippen Method
logp	8.434		Crippen Method
mvol	408.740	ml/mol	McGowan Method
pc	808.91	kPa	Joback Method
rinpol	3159.00		NIST Webbook
rinpol	3159.00		NIST Webbook
tb	1058.48	K	Joback Method
tc	1299.92	K	Joback Method
tf	620.92	K	Joback Method
vc	1.581	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1395.04	J/molxK	1058.48	Joback Method
cpg	1412.19	J/molxK	1098.72	Joback Method
cpg	1427.77	J/molxK	1138.96	Joback Method
cpg	1441.87	J/molxK	1179.20	Joback Method
cpg	1454.61	J/molxK	1219.44	Joback Method
cpg	1466.09	J/molxK	1259.68	Joback Method
cpg	1476.43	J/molxK	1299.92	Joback Method
dvisc	0.0001564	Paxs	620.92	Joback Method

dvisc	0.0000784	Paxs	693.85	Joback Method
dvisc	0.0000449	Paxs	766.77	Joback Method
dvisc	0.0000283	Paxs	839.70	Joback Method
dvisc	0.0000192	Paxs	912.63	Joback Method
dvisc	0.0000138	Paxs	985.55	Joback Method
dvisc	0.0000104	Paxs	1058.48	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=U369353&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369353&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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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