

# Diethylmalonic acid, monochloride, 3-chlorobenzyl ester

<b>Inchi:</b>	InChI=1S/C14H16Cl2O3/c1-3-14(4-2,12(16)17)13(18)19-9-10-6-5-7-11(15)8-10/h5-8H,3
<b>InchiKey:</b>	KSCQBHVFCRFB-UHFFFAOYSA-N
<b>Formula:</b>	C14H16Cl2O3
<b>SMILES:</b>	CCC(CC)(C(=O)Cl)C(=O)OCc1cccc(Cl)c1
<b>Mol. weight [g/mol]:</b>	303.18

## Physical Properties

Property code	Value	Unit	Source
gf	-214.08	kJ/mol	Joback Method
hf	-504.84	kJ/mol	Joback Method
hfus	31.03	kJ/mol	Joback Method
hvap	73.07	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.955		Crippen Method
mcvol	217.850	ml/mol	McGowan Method
pc	2081.22	kPa	Joback Method
rmpol	1934.00		NIST Webbook
tb	753.17	K	Joback Method
tc	977.79	K	Joback Method
tf	470.83	K	Joback Method
vc	0.829	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.97	J/molxK	753.17	Joback Method
cpg	579.78	J/molxK	790.61	Joback Method
cpg	591.60	J/molxK	828.04	Joback Method
cpg	602.47	J/molxK	865.48	Joback Method
cpg	612.45	J/molxK	902.92	Joback Method
cpg	621.60	J/molxK	940.35	Joback Method
cpg	629.96	J/molxK	977.79	Joback Method
dvisc	0.0009599	Paxs	470.83	Joback Method
dvisc	0.0005583	Paxs	517.89	Joback Method

dvisc	0.0003554	Paxs	564.94	Joback Method
dvisc	0.0002425	Paxs	612.00	Joback Method
dvisc	0.0001747	Paxs	659.06	Joback Method
dvisc	0.0001315	Paxs	706.11	Joback Method
dvisc	0.0001026	Paxs	753.17	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=U369359&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369359&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>mccvol:</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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