

# Diethylmalonic acid, monochloride, 2-hexyl ester

Inchi:	InChI=1S/C13H23ClO3/c1-5-8-9-10(4)17-12(16)13(6-2,7-3)11(14)15/h10H,5-9H2,1-4H3
InchiKey:	AIYXBPLQLSQRIQ-UHFFFAOYSA-N
Formula:	C13H23ClO3
SMILES:	CCCCC(C)OC(=O)C(CC)(CC)C(=O)Cl
Mol. weight [g/mol]:	262.77

## Physical Properties

Property code	Value	Unit	Source
gf	-315.79	kJ/mol	Joback Method
hf	-698.80	kJ/mol	Joback Method
hfus	27.07	kJ/mol	Joback Method
hvap	63.14	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.680		Crippen Method
mcvol	215.280	ml/mol	McGowan Method
pc	1784.86	kPa	Joback Method
rinpol	1448.00		NIST Webbook
rinpol	1448.00		NIST Webbook
tb	660.76	K	Joback Method
tc	852.92	K	Joback Method
tf	375.70	K	Joback Method
vc	0.826	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.05	J/mol×K	660.76	Joback Method
cpg	642.21	J/mol×K	820.90	Joback Method
cpg	630.17	J/mol×K	788.87	Joback Method
cpg	617.36	J/mol×K	756.84	Joback Method
cpg	603.76	J/mol×K	724.81	Joback Method
cpg	589.33	J/mol×K	692.79	Joback Method
cpg	653.51	J/mol×K	852.92	Joback Method
dvisc	0.0001266	Paxs	660.76	Joback Method

dvisc	0.0001716	Paxs	613.25	Joback Method
dvisc	0.0002450	Paxs	565.74	Joback Method
dvisc	0.0003733	Paxs	518.23	Joback Method
dvisc	0.0006192	Paxs	470.72	Joback Method
dvisc	0.0011508	Paxs	423.21	Joback Method
dvisc	0.0025016	Paxs	375.70	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=U370638&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370638&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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