

# Diethylmalonic acid, monochloride, 4-methylpent-2-yl ester

<b>Inchi:</b>	InChI=1S/C13H23ClO3/c1-6-13(7-2,11(14)15)12(16)17-10(5)8-9(3)4/h9-10H,6-8H2,1-5H
<b>InchiKey:</b>	HTDWBWLHGHSCFP-UHFFFAOYSA-N
<b>Formula:</b>	C13H23ClO3
<b>SMILES:</b>	CCC(CC)(C(=O)Cl)C(=O)OC(C)CC(C)C
<b>Mol. weight [g/mol]:</b>	262.77

## Physical Properties

Property code	Value	Unit	Source
gf	-318.23	kJ/mol	Joback Method
hf	-704.08	kJ/mol	Joback Method
hfus	23.55	kJ/mol	Joback Method
hvap	62.75	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.536		Crippen Method
mcvol	215.280	ml/mol	McGowan Method
pc	1796.98	kPa	Joback Method
rinqol	1406.00		NIST Webbook
tb	660.32	K	Joback Method
tc	855.72	K	Joback Method
tf	360.70	K	Joback Method
vc	0.820	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.52	J/molxK	660.32	Joback Method
cpg	590.10	J/molxK	692.89	Joback Method
cpg	604.78	J/molxK	725.45	Joback Method
cpg	618.59	J/molxK	758.02	Joback Method
cpg	631.58	J/molxK	790.59	Joback Method
cpg	643.77	J/molxK	823.16	Joback Method
cpg	655.19	J/molxK	855.72	Joback Method
dvisc	0.0032395	Paxs	360.70	Joback Method
dvisc	0.0013318	Paxs	410.64	Joback Method

dvisc	0.0006639	Paxs	460.57	Joback Method
dvisc	0.0003793	Paxs	510.51	Joback Method
dvisc	0.0002394	Paxs	560.45	Joback Method
dvisc	0.0001629	Paxs	610.38	Joback Method
dvisc	0.0001175	Paxs	660.32	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=U370503&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370503&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>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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