

# Diethylmalonic acid, di(4-chlorophenyl) ester

<b>Inchi:</b>	InChI=1S/C19H18Cl2O4/c1-3-19(4-2,17(22)24-15-9-5-13(20)6-10-15)18(23)25-16-11-7-
<b>InchiKey:</b>	MSPOUWXGWYMYMK-UHFFFAOYSA-N
<b>Formula:</b>	C19H18Cl2O4
<b>SMILES:</b>	CCC(CC)(C(=O)Oc1ccc(Cl)cc1)C(=O)Oc1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	381.25

## Physical Properties

Property code	Value	Unit	Source
gf	-174.20	kJ/mol	Joback Method
hf	-515.20	kJ/mol	Joback Method
hfus	38.82	kJ/mol	Joback Method
hvap	89.55	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	5.311		Crippen Method
mcvol	270.410	ml/mol	McGowan Method
pc	1775.84	kPa	Joback Method
rinpol	2578.00		NIST Webbook
tb	921.65	K	Joback Method
tc	1163.19	K	Joback Method
tf	588.35	K	Joback Method
vc	1.018	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.29	J/molxK	921.65	Joback Method
cpg	779.75	J/molxK	961.91	Joback Method
cpg	789.99	J/molxK	1002.16	Joback Method
cpg	799.08	J/molxK	1042.42	Joback Method
cpg	807.09	J/molxK	1082.68	Joback Method
cpg	814.09	J/molxK	1122.94	Joback Method
cpg	820.14	J/molxK	1163.19	Joback Method
dvisc	0.0003021	Paxs	588.35	Joback Method
dvisc	0.0001840	Paxs	643.90	Joback Method

dvisc	0.0001212	Paxs	699.45	Joback Method
dvisc	0.0000849	Paxs	755.00	Joback Method
dvisc	0.0000624	Paxs	810.55	Joback Method
dvisc	0.0000478	Paxs	866.10	Joback Method
dvisc	0.0000378	Paxs	921.65	Joback Method

## Sources

<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=U369907&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369907&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>

## 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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