

# Diethylmalonic acid, 2-chloro-5-methylphenyl pentyl ester

Inchi:	InChI=1S/C19H27ClO4/c1-5-8-9-12-23-17(21)19(6-2,7-3)18(22)24-16-13-14(4)10-11-15
InchiKey:	HDMLRBKBZYBXEN-UHFFFAOYSA-N
Formula:	C19H27ClO4
SMILES:	CCCCCOC(=O)C(CC)(CC)C(=O)Oc1cc(C)ccc1Cl
Mol. weight [g/mol]:	354.87

## Physical Properties

Property code	Value	Unit	Source
gf	-274.68	kJ/mol	Joback Method
hf	-735.99	kJ/mol	Joback Method
hfus	40.59	kJ/mol	Joback Method
hvap	82.89	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	5.094		Crippen Method
mcvol	281.930	ml/mol	McGowan Method
pc	1405.90	kPa	Joback Method
rinsol	2245.00		NIST Webbook
tb	857.54	K	Joback Method
tc	1068.20	K	Joback Method
tf	532.01	K	Joback Method
vc	1.077	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.41	J/molxK	857.54	Joback Method
cpg	909.65	J/molxK	1033.09	Joback Method
cpg	899.09	J/molxK	997.98	Joback Method
cpg	887.53	J/molxK	962.87	Joback Method
cpg	874.92	J/molxK	927.76	Joback Method
cpg	861.22	J/molxK	892.65	Joback Method
cpg	919.23	J/molxK	1068.20	Joback Method
dvisc	0.0000435	Paxs	857.54	Joback Method
dvisc	0.0000559	Paxs	803.28	Joback Method

dvisc	0.0000745	Paxs	749.03	Joback Method
dvisc	0.0001037	Paxs	694.77	Joback Method
dvisc	0.0001528	Paxs	640.52	Joback Method
dvisc	0.0002419	Paxs	586.26	Joback Method
dvisc	0.0004205	Paxs	532.01	Joback Method

## Sources

<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>
<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=U370455&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370455&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>

## 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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