

# Diethylmalonic acid, 3,5-dichlorophenyl hexyl ester

Inchi:	InChI=1S/C19H26Cl2O4/c1-4-7-8-9-10-24-17(22)19(5-2,6-3)18(23)25-16-12-14(20)11-15
InchiKey:	SUOTWPCEJZSEPV-UHFFFAOYSA-N
Formula:	C19H26Cl2O4
SMILES:	CCCCCOC(=O)C(CC)(CC)C(=O)Oc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]:	389.31

## Physical Properties

Property code	Value	Unit	Source
gf	-286.61	kJ/mol	Joback Method
hf	-751.73	kJ/mol	Joback Method
hfus	44.78	kJ/mol	Joback Method
hvap	87.27	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	5.829		Crippen Method
mvol	294.170	ml/mol	McGowan Method
pc	1367.69	kPa	Joback Method
rinpol	2348.00		NIST Webbook
rinpol	2348.00		NIST Webbook
tb	894.97	K	Joback Method
tc	1110.14	K	Joback Method
tf	561.93	K	Joback Method
vc	1.127	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.23	J/molxK	894.97	Joback Method
cpg	928.59	J/molxK	1074.28	Joback Method
cpg	919.18	J/molxK	1038.42	Joback Method
cpg	908.78	J/molxK	1002.56	Joback Method
cpg	897.35	J/molxK	966.69	Joback Method
cpg	884.85	J/molxK	930.83	Joback Method
cpg	937.05	J/molxK	1110.14	Joback Method
dvisc	0.0000369	Paxs	894.97	Joback Method

dvisc	0.0000473	Paxs	839.46	Joback Method
dvisc	0.0000627	Paxs	783.96	Joback Method
dvisc	0.0000868	Paxs	728.45	Joback Method
dvisc	0.0001269	Paxs	672.94	Joback Method
dvisc	0.0001985	Paxs	617.44	Joback Method
dvisc	0.0003392	Paxs	561.93	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U370440&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370440&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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