

# Diethylmalonic acid, nonyl 2,3,5-trichlorophenyl ester

Inchi:	InChI=1S/C22H31Cl3O4/c1-4-7-8-9-10-11-12-13-28-20(26)22(5-2,6-3)21(27)29-18-15-16
InchiKey:	ZAUXYBZUHWBDHD-UHFFFAOYSA-N
Formula:	C22H31Cl3O4
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cc(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	465.84

## Physical Properties

Property code	Value	Unit	Source
gf	-282.91	kJ/mol	Joback Method
hf	-840.86	kJ/mol	Joback Method
hfus	56.36	kJ/mol	Joback Method
hvap	99.00	kJ/mol	Joback Method
log10ws	-8.32		Crippen Method
logp	7.652		Crippen Method
mvol	348.680	ml/mol	McGowan Method
pc	1079.22	kPa	Joback Method
rinpol	2806.00		NIST Webbook
tb	1006.02	K	Joback Method
tc	1232.99	K	Joback Method
tf	638.18	K	Joback Method
vc	1.343	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1070.18	J/molxK	1006.02	Joback Method
cpg	1122.99	J/molxK	1195.16	Joback Method
cpg	1114.70	J/molxK	1157.33	Joback Method
cpg	1105.33	J/molxK	1119.51	Joback Method
cpg	1094.83	J/molxK	1081.68	Joback Method
cpg	1083.13	J/molxK	1043.85	Joback Method
cpg	1130.26	J/molxK	1232.99	Joback Method
dvisc	0.0000196	Paxs	1006.02	Joback Method
dvisc	0.0000250	Paxs	944.71	Joback Method

dvisc	0.0000330	Paxs	883.41	Joback Method
dvisc	0.0000452	Paxs	822.10	Joback Method
dvisc	0.0000654	Paxs	760.79	Joback Method
dvisc	0.0001007	Paxs	699.49	Joback Method
dvisc	0.0001686	Paxs	638.18	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=U370551&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370551&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>mccvol:</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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