

# Diethylmalonic acid, dodecyl 2,4,5-trichlorophenyl ester

Inchi:	InChI=1S/C25H37Cl3O4/c1-4-7-8-9-10-11-12-13-14-15-16-31-23(29)25(5-2,6-3)24(30)32
InchiKey:	ZYNLKTVPCORZII-UHFFFAOYSA-N
Formula:	C25H37Cl3O4
SMILES:	CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	507.92

## Physical Properties

Property code	Value	Unit	Source
gf	-257.65	kJ/mol	Joback Method
hf	-902.78	kJ/mol	Joback Method
hfus	64.13	kJ/mol	Joback Method
hvap	105.68	kJ/mol	Joback Method
log10ws	-9.58		Crippen Method
logp	8.823		Crippen Method
mcvol	390.950	ml/mol	McGowan Method
pc	900.72	kPa	Joback Method
rinpol	3141.00		NIST Webbook
rinpol	3141.00		NIST Webbook
tb	1074.66	K	Joback Method
tc	1316.85	K	Joback Method
tf	671.99	K	Joback Method
vc	1.512	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1252.13	J/molxK	1074.66	Joback Method
cpg	1306.83	J/molxK	1276.49	Joback Method
cpg	1298.45	J/molxK	1236.12	Joback Method
cpg	1288.87	J/molxK	1195.76	Joback Method
cpg	1278.01	J/molxK	1155.39	Joback Method
cpg	1265.79	J/molxK	1115.03	Joback Method
cpg	1314.10	J/molxK	1316.85	Joback Method
dvisc	0.0000121	Paxs	1074.66	Joback Method

dvisc	0.0000155	Paxs	1007.55	Joback Method
dvisc	0.0000206	Paxs	940.44	Joback Method
dvisc	0.0000287	Paxs	873.32	Joback Method
dvisc	0.0000422	Paxs	806.21	Joback Method
dvisc	0.0000664	Paxs	739.10	Joback Method
dvisc	0.0001146	Paxs	671.99	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U370539&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370539&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>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</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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