

# Dimethylmalonic acid, pentyl 2,4,6-trichlorophenyl ester

<b>Inchi:</b>	InChI=1S/C16H19Cl3O4/c1-4-5-6-7-22-14(20)16(2,3)15(21)23-13-11(18)8-10(17)9-12(13)
<b>InchiKey:</b>	RKWSHNYQJPOSJJ-UHFFFAOYSA-N
<b>Formula:</b>	C16H19Cl3O4
<b>SMILES:</b>	CCCCCOC(=O)C(C)(C)C(=O)Oc1c(Cl)cc(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	381.68

## Physical Properties

Property code	Value	Unit	Source
gf	-333.43	kJ/mol	Joback Method
hf	-717.02	kJ/mol	Joback Method
hfus	40.82	kJ/mol	Joback Method
hvap	85.64	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.312		Crippen Method
mcvol	264.140	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
rinpol	2262.00		NIST Webbook
tb	868.74	K	Joback Method
tc	1090.97	K	Joback Method
tf	570.56	K	Joback Method
vc	1.008	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.62	J/molxK	868.74	Joback Method
cpg	770.05	J/molxK	1053.93	Joback Method
cpg	762.30	J/molxK	1016.89	Joback Method
cpg	753.61	J/molxK	979.86	Joback Method
cpg	743.96	J/molxK	942.82	Joback Method
cpg	733.30	J/molxK	905.78	Joback Method
cpg	776.89	J/molxK	1090.97	Joback Method
dvisc	0.0000500	Paxs	868.74	Joback Method
dvisc	0.0000624	Paxs	819.04	Joback Method

dvisc	0.0000803	Paxs	769.35	Joback Method
dvisc	0.0001069	Paxs	719.65	Joback Method
dvisc	0.0001484	Paxs	669.95	Joback Method
dvisc	0.0002173	Paxs	620.26	Joback Method
dvisc	0.0003400	Paxs	570.56	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U363648&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U363648&amp;Units=SI</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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