

# Dimethylmalonic acid, 2,5-dichlorophenyl octadecyl ester

Inchi:	InChI=1S/C29H46Cl2O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-34-27(32)29
InchiKey:	QGIBKIZWWXPTGZ-UHFFFAOYSA-N
Formula:	C29H46Cl2O4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1cc(Cl)ccc1Cl
Mol. weight [g/mol]:	529.58

## Physical Properties

Property code	Value	Unit	Source
gf	-202.41	kJ/mol	Joback Method
hf	-958.13	kJ/mol	Joback Method
hfus	70.68	kJ/mol	Joback Method
hvap	109.53	kJ/mol	Joback Method
log10ws	-10.57		Crippen Method
logp	9.730		Crippen Method
mcvol	435.070	ml/mol	McGowan Method
pc	744.88	kPa	Joback Method
rinpol	3437.00		NIST Webbook
rinpol	3437.00		NIST Webbook
tb	1123.77	K	Joback Method
tc	1388.35	K	Joback Method
tf	674.63	K	Joback Method
vc	1.687	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1480.41	J/molxK	1123.77	Joback Method
cpg	1496.77	J/molxK	1167.87	Joback Method
cpg	1511.37	J/molxK	1211.96	Joback Method
cpg	1524.35	J/molxK	1256.06	Joback Method
cpg	1535.86	J/molxK	1300.16	Joback Method
cpg	1546.03	J/molxK	1344.25	Joback Method
cpg	1555.00	J/molxK	1388.35	Joback Method
dvisc	0.0000941	Paxs	674.63	Joback Method

dvisc	0.0000498	Paxs	749.49	Joback Method
dvisc	0.0000296	Paxs	824.34	Joback Method
dvisc	0.0000192	Paxs	899.20	Joback Method
dvisc	0.0000133	Paxs	974.06	Joback Method
dvisc	0.0000097	Paxs	1048.91	Joback Method
dvisc	0.0000074	Paxs	1123.77	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=U363695&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U363695&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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