

# Dimethylmalonic acid, 2,4-dichloro-6-formylphenyl heptyl ester

Inchi:	InChI=1S/C19H24Cl2O5/c1-4-5-6-7-8-9-25-17(23)19(2,3)18(24)26-16-13(12-22)10-14(20)
InchiKey:	UZWAIVLKTPSFAN-UHFFFAOYSA-N
Formula:	C19H24Cl2O5
SMILES:	CCCCCCCOC(=O)C(C)(C)C(=O)Oc1c(Cl)cc(Cl)cc1C=O
Mol. weight [g/mol]:	403.30

## Physical Properties

Property code	Value	Unit	Source
gf	-395.76	kJ/mol	Joback Method
hf	-848.78	kJ/mol	Joback Method
hfus	46.68	kJ/mol	Joback Method
hvap	94.66	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.251		Crippen Method
mvol	295.740	ml/mol	McGowan Method
pc	1429.38	kPa	Joback Method
rinpol	2532.00		NIST Webbook
rinpol	2532.00		NIST Webbook
tb	948.61	K	Joback Method
tc	1170.08	K	Joback Method
tf	616.45	K	Joback Method
vc	1.143	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.83	J/molxK	948.61	Joback Method
cpg	891.48	J/molxK	985.52	Joback Method
cpg	902.00	J/molxK	1022.43	Joback Method
cpg	911.43	J/molxK	1059.35	Joback Method
cpg	919.81	J/molxK	1096.26	Joback Method
cpg	927.17	J/molxK	1133.17	Joback Method
cpg	933.56	J/molxK	1170.08	Joback Method
dvisc	0.0002883	Paxs	616.45	Joback Method

dvisc	0.0001808	Paxs	671.81	Joback Method
dvisc	0.0001217	Paxs	727.17	Joback Method
dvisc	0.0000867	Paxs	782.53	Joback Method
dvisc	0.0000645	Paxs	837.89	Joback Method
dvisc	0.0000498	Paxs	893.25	Joback Method
dvisc	0.0000397	Paxs	948.61	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=U363636&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U363636&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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