

# Dimethyl 1,3,3,3-tetrachloro-2-oxopropylmalonate

Inchi:	InChI=1S/C8H8Cl4O5/c1-16-6(14)3(7(15)17-2)4(9)5(13)8(10,11)12/h3-4H,1-2H3
InchiKey:	QGVYOOAIJUVSHJ-UHFFFAOYSA-N
Formula:	C8H8Cl4O5
SMILES:	COC(=O)C(C(=O)OC)C(Cl)C(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	325.96

## Physical Properties

Property code	Value	Unit	Source
gf	-630.04	kJ/mol	Joback Method
hf	-892.90	kJ/mol	Joback Method
hfus	25.98	kJ/mol	Joback Method
hvap	73.93	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.495		Crippen Method
mcvol	188.990	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
rinpol	1569.00		NIST Webbook
rinpol	1569.00		NIST Webbook
tb	734.50	K	Joback Method
tc	958.76	K	Joback Method
tf	466.27	K	Joback Method
vc	0.711	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.36	J/molxK	734.50	Joback Method
cpg	437.52	J/molxK	771.88	Joback Method
cpg	444.93	J/molxK	809.25	Joback Method
cpg	451.62	J/molxK	846.63	Joback Method
cpg	457.58	J/molxK	884.01	Joback Method
cpg	462.85	J/molxK	921.39	Joback Method
cpg	467.44	J/molxK	958.76	Joback Method
dvisc	0.0012145	Paxs	466.27	Joback Method

dvisc	0.0006855	Paxs	510.97	Joback Method
dvisc	0.0004243	Paxs	555.68	Joback Method
dvisc	0.0002820	Paxs	600.38	Joback Method
dvisc	0.0001984	Paxs	645.09	Joback Method
dvisc	0.0001460	Paxs	689.80	Joback Method
dvisc	0.0001116	Paxs	734.50	Joback Method

## Sources

<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=R80198&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R80198&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>

## 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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