

# Malonic acid, 2,2-dichloroethyl octyl ester

<b>Inchi:</b>	InChI=1S/C13H22Cl2O4/c1-2-3-4-5-6-7-8-18-12(16)9-13(17)19-10-11(14)15/h11H,2-10H
<b>InchiKey:</b>	PLAYDBGXBJBHEE-UHFFFAOYSA-N
<b>Formula:</b>	C13H22Cl2O4
<b>SMILES:</b>	CCCCCCCCOC(=O)CC(=O)OCC(Cl)Cl
<b>Mol. weight [g/mol]:</b>	313.22

## Physical Properties

Property code	Value	Unit	Source
gf	-435.56	kJ/mol	Joback Method
hf	-838.01	kJ/mol	Joback Method
hfus	39.87	kJ/mol	Joback Method
hvap	71.23	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.627		Crippen Method
mcvol	233.390	ml/mol	McGowan Method
pc	1679.66	kPa	Joback Method
rinpola	1959.00		NIST Webbook
tb	723.84	K	Joback Method
tc	911.74	K	Joback Method
tf	425.43	K	Joback Method
vc	0.903	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.11	J/molxK	723.84	Joback Method
cpg	640.84	J/molxK	755.16	Joback Method
cpg	653.80	J/molxK	786.47	Joback Method
cpg	666.00	J/molxK	817.79	Joback Method
cpg	677.44	J/molxK	849.10	Joback Method
cpg	688.12	J/molxK	880.42	Joback Method
cpg	698.07	J/molxK	911.74	Joback Method
dvisc	0.0012999	Paxs	425.43	Joback Method
dvisc	0.0006770	Paxs	475.16	Joback Method

dvisc	0.0003990	Paxs	524.90	Joback Method
dvisc	0.0002577	Paxs	574.63	Joback Method
dvisc	0.0001784	Paxs	624.37	Joback Method
dvisc	0.0001304	Paxs	674.10	Joback Method
dvisc	0.0000995	Paxs	723.84	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U349063&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U349063&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>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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