

# Fumaric acid, 2,2-dichloroethyl tridecyl ester

<b>Inchi:</b>	InChI=1S/C19H32Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-12-15-24-18(22)13-14-19(23)25-16-17
<b>InchiKey:</b>	XEUKCOQEWZJXBR-BUHFOSPRSA-N
<b>Formula:</b>	C19H32Cl2O4
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)C=CC(=O)OCC(Cl)Cl
<b>Mol. weight [g/mol]:</b>	395.36

## Physical Properties

Property code	Value	Unit	Source
gf	-304.82	kJ/mol	Joback Method
hf	-844.63	kJ/mol	Joback Method
hfus	55.61	kJ/mol	Joback Method
hvap	84.54	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.744		Crippen Method
mvol	313.630	ml/mol	McGowan Method
pc	1138.27	kPa	Joback Method
rinpol	2632.00		NIST Webbook
rinpol	2632.00		NIST Webbook
tb	865.28	K	Joback Method
tc	1062.58	K	Joback Method
tf	487.97	K	Joback Method
vc	1.220	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	943.77	J/molxK	865.28	Joback Method
cpg	1011.59	J/molxK	1029.70	Joback Method
cpg	999.92	J/molxK	996.82	Joback Method
cpg	987.34	J/molxK	963.93	Joback Method
cpg	973.81	J/molxK	931.05	Joback Method
cpg	959.30	J/molxK	898.16	Joback Method
cpg	1022.38	J/molxK	1062.58	Joback Method
dvisc	0.0000359	Paxs	865.28	Joback Method

dvisc	0.0000479	Paxs	802.39	Joback Method
dvisc	0.0000672	Paxs	739.51	Joback Method
dvisc	0.0001004	Paxs	676.62	Joback Method
dvisc	0.0001628	Paxs	613.74	Joback Method
dvisc	0.0002948	Paxs	550.86	Joback Method
dvisc	0.0006222	Paxs	487.97	Joback Method

## Sources

<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=U348581&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348581&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> 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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