

# Fumaric acid, 2-chloropropyl nonyl ester

<b>Inchi:</b>	InChI=1S/C16H27ClO4/c1-3-4-5-6-7-8-9-12-20-15(18)10-11-16(19)21-13-14(2)17/h10-11
<b>InchiKey:</b>	CPJZMLBWUCJYLQ-ZHACJKMWSA-N
<b>Formula:</b>	C16H27ClO4
<b>SMILES:</b>	CCCCCCCCCOC(=O)C=CC(=O)OCC(C)Cl
<b>Mol. weight [g/mol]:</b>	318.84

## Physical Properties

Property code	Value	Unit	Source
gf	-318.15	kJ/mol	Joback Method
hf	-766.97	kJ/mol	Joback Method
hfus	43.65	kJ/mol	Joback Method
hvap	73.48	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.007		Crippen Method
mcvol	259.120	ml/mol	McGowan Method
pc	1435.89	kPa	Joback Method
rinpol	2169.00		NIST Webbook
tb	759.21	K	Joback Method
tc	946.71	K	Joback Method
tf	424.24	K	Joback Method
vc	1.002	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.99	J/molxK	759.21	Joback Method
cpg	809.35	J/molxK	915.46	Joback Method
cpg	797.32	J/molxK	884.21	Joback Method
cpg	784.49	J/molxK	852.96	Joback Method
cpg	770.83	J/molxK	821.71	Joback Method
cpg	756.34	J/molxK	790.46	Joback Method
cpg	820.60	J/molxK	946.71	Joback Method
dvisc	0.0000650	Paxs	759.21	Joback Method
dvisc	0.0000865	Paxs	703.38	Joback Method

dvisc	0.0001210	Paxs	647.55	Joback Method
dvisc	0.0001804	Paxs	591.72	Joback Method
dvisc	0.0002921	Paxs	535.90	Joback Method
dvisc	0.0005293	Paxs	480.07	Joback Method
dvisc	0.0011214	Paxs	424.24	Joback Method

## Sources

<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=U348567&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348567&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>

## 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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