

# Fumaric acid, 2-chlorophenyl 2-ethylhexyl ester

Inchi:	InChI=1S/C18H23ClO4/c1-3-5-8-14(4-2)13-22-17(20)11-12-18(21)23-16-10-7-6-9-15(16)
InchiKey:	OSCMBMNZFREGEI-VAWYXSNFSA-N
Formula:	C18H23ClO4
SMILES:	CCCCC(CC)COC(=O)C=CC(=O)Oc1ccccc1Cl
Mol. weight [g/mol]:	338.83

## Physical Properties

Property code	Value	Unit	Source
gf	-198.53	kJ/mol	Joback Method
hf	-583.19	kJ/mol	Joback Method
hfus	42.48	kJ/mol	Joback Method
hvap	80.87	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.561		Crippen Method
mvol	263.540	ml/mol	McGowan Method
pc	1580.97	kPa	Joback Method
rinpol	2349.00		NIST Webbook
rinpol	2349.00		NIST Webbook
tb	836.63	K	Joback Method
tc	1048.04	K	Joback Method
tf	485.72	K	Joback Method
vc	1.006	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.42	J/molxK	836.63	Joback Method
cpg	776.62	J/molxK	871.86	Joback Method
cpg	789.77	J/molxK	907.10	Joback Method
cpg	801.91	J/molxK	942.33	Joback Method
cpg	813.06	J/molxK	977.57	Joback Method
cpg	823.27	J/molxK	1012.80	Joback Method
cpg	832.56	J/molxK	1048.04	Joback Method
dvisc	0.0006195	Paxs	485.72	Joback Method

dvisc	0.0003254	Paxs	544.21	Joback Method
dvisc	0.0001937	Paxs	602.69	Joback Method
dvisc	0.0001264	Paxs	661.17	Joback Method
dvisc	0.0000884	Paxs	719.66	Joback Method
dvisc	0.0000652	Paxs	778.14	Joback Method
dvisc	0.0000502	Paxs	836.63	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=U405725&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405725&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>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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