

# Fumaric acid, 2-octyl 8-chlorooctyl ester

**Inchi:** InChI=1S/C20H35ClO4/c1-3-4-5-10-13-18(2)25-20(23)15-14-19(22)24-17-12-9-7-6-8-11-12  
**InchiKey:** LKOHSJLXLOGH MV-CCEZHUSRSA-N  
**Formula:** C20H35ClO4  
**SMILES:** CCCCCC(C)OC(=O)C=CC(=O)OCCCCCCCCCl  
**Mol. weight [g/mol]:** 374.94

## Physical Properties

Property code	Value	Unit	Source
gf	-284.47	kJ/mol	Joback Method
hf	-849.53	kJ/mol	Joback Method
hfus	54.01	kJ/mol	Joback Method
hvap	82.38	kJ/mol	Joback Method
log10ws	-6.04		Crippen Method
logp	5.567		Crippen Method
mvol	315.480	ml/mol	McGowan Method
pc	1094.27	kPa	Joback Method
rinpol	2595.00		NIST Webbook
rinpol	2595.00		NIST Webbook
tb	850.73	K	Joback Method
tc	1044.27	K	Joback Method
tf	469.32	K	Joback Method
vc	1.226	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	975.00	J/molxK	850.73	Joback Method
cpg	991.85	J/molxK	882.99	Joback Method
cpg	1007.65	J/molxK	915.24	Joback Method
cpg	1022.43	J/molxK	947.50	Joback Method
cpg	1036.24	J/molxK	979.76	Joback Method
cpg	1049.09	J/molxK	1012.02	Joback Method
cpg	1061.03	J/molxK	1044.27	Joback Method
dvisc	0.0007139	Paxs	469.32	Joback Method

dvisc	0.0003234	Paxs	532.89	Joback Method
dvisc	0.0001734	Paxs	596.46	Joback Method
dvisc	0.0001049	Paxs	660.02	Joback Method
dvisc	0.0000693	Paxs	723.59	Joback Method
dvisc	0.0000489	Paxs	787.16	Joback Method
dvisc	0.0000364	Paxs	850.73	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U405592&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405592&amp;Units=SI</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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