

# Fumaric acid, 4-chlorophenyl 8-chlorooctyl ester

<b>Inchi:</b>	InChI=1S/C18H22Cl2O4/c19-13-5-3-1-2-4-6-14-23-17(21)11-12-18(22)24-16-9-7-15(20)
<b>InchiKey:</b>	KOKFVOREEYHZOP-VAWYXSNFSA-N
<b>Formula:</b>	C18H22Cl2O4
<b>SMILES:</b>	O=C(C=CC(=O)Oc1ccc(Cl)cc1)OCCCCCCCCCl
<b>Mol. weight [g/mol]:</b>	373.27

## Physical Properties

Property code	Value	Unit	Source
gf	-208.02	kJ/mol	Joback Method
hf	-593.65	kJ/mol	Joback Method
hfus	50.20	kJ/mol	Joback Method
hvap	85.64	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	4.924		Crippen Method
mcvol	275.780	ml/mol	McGowan Method
pc	1525.88	kPa	Joback Method
rinpol	2811.00		NIST Webbook
rinpol	2811.00		NIST Webbook
tb	874.50	K	Joback Method
tc	1087.79	K	Joback Method
tf	530.64	K	Joback Method
vc	1.062	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	786.17	J/molxK	874.50	Joback Method
cpg	799.10	J/molxK	910.05	Joback Method
cpg	811.02	J/molxK	945.60	Joback Method
cpg	821.97	J/molxK	981.14	Joback Method
cpg	831.99	J/molxK	1016.69	Joback Method
cpg	841.12	J/molxK	1052.24	Joback Method
cpg	849.39	J/molxK	1087.79	Joback Method
dvisc	0.0004505	Paxs	530.64	Joback Method

dvisc	0.0002576	Paxs	587.95	Joback Method
dvisc	0.0001627	Paxs	645.26	Joback Method
dvisc	0.0001107	Paxs	702.57	Joback Method
dvisc	0.0000799	Paxs	759.88	Joback Method
dvisc	0.0000603	Paxs	817.19	Joback Method
dvisc	0.0000472	Paxs	874.50	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=U405847&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405847&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>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>h<sub>vap</sub>:</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>log<sub>p</sub>:</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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