

# Fumaric acid, 4-methoxyphenyl 8-chlorooctyl ester

Inchi:	InChI=1S/C19H25ClO5/c1-23-16-8-10-17(11-9-16)25-19(22)13-12-18(21)24-15-7-5-3-2-4
InchiKey:	WXBNGDVCNJWEHF-OUKQBFOZSA-N
Formula:	C19H25ClO5
SMILES:	COc1ccc(OC(=O)C=CC(=O)OCCCCCCCCCl)cc1
Mol. weight [g/mol]:	368.85

## Physical Properties

Property code	Value	Unit	Source
gf	-292.67	kJ/mol	Joback Method
hf	-730.77	kJ/mol	Joback Method
hfus	49.78	kJ/mol	Joback Method
hvap	85.89	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.279		Crippen Method
mvol	283.500	ml/mol	McGowan Method
pc	1439.16	kPa	Joback Method
rinpol	2904.00		NIST Webbook
rinpol	2904.00		NIST Webbook
tb	882.37	K	Joback Method
tc	1091.85	K	Joback Method
tf	534.22	K	Joback Method
vc	1.087	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	847.19	J/molxK	882.37	Joback Method
cpg	905.14	J/molxK	1056.94	Joback Method
cpg	895.71	J/molxK	1022.03	Joback Method
cpg	885.22	J/molxK	987.11	Joback Method
cpg	873.66	J/molxK	952.20	Joback Method
cpg	860.98	J/molxK	917.28	Joback Method
cpg	913.54	J/molxK	1091.85	Joback Method
dvisc	0.0000356	Paxs	882.37	Joback Method

dvisc	0.0000455	Paxs	824.34	Joback Method
dvisc	0.0000605	Paxs	766.32	Joback Method
dvisc	0.0000841	Paxs	708.29	Joback Method
dvisc	0.0001241	Paxs	650.27	Joback Method
dvisc	0.0001977	Paxs	592.25	Joback Method
dvisc	0.0003483	Paxs	534.22	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=U405783&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405783&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>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rin<sub>pol</sub>:</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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