

# Fumaric acid, 4-chlorophenyl 3-methylbut-2-yl ester

Inchi:	InChI=1S/C15H17ClO4/c1-10(2)11(3)19-14(17)8-9-15(18)20-13-6-4-12(16)5-7-13/h4-11H
InchiKey:	MNNQONZPGLFYBU-CMDGGGOBGSA-N
Formula:	C15H17ClO4
SMILES:	CC(C)C(C)OC(=O)C=CC(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]:	296.75

## Physical Properties

Property code	Value	Unit	Source
gf	-226.23	kJ/mol	Joback Method
hf	-526.55	kJ/mol	Joback Method
hfus	31.18	kJ/mol	Joback Method
hvap	73.80	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.389		Crippen Method
mcvol	221.270	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinpol	2057.00		NIST Webbook
rinpol	2057.00		NIST Webbook
tb	767.55	K	Joback Method
tc	988.14	K	Joback Method
tf	436.91	K	Joback Method
vc	0.833	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.13	J/molxK	767.55	Joback Method
cpg	654.04	J/molxK	951.37	Joback Method
cpg	644.38	J/molxK	914.61	Joback Method
cpg	633.79	J/molxK	877.84	Joback Method
cpg	622.24	J/molxK	841.08	Joback Method
cpg	609.70	J/molxK	804.31	Joback Method
cpg	662.79	J/molxK	988.14	Joback Method
dvisc	0.0000695	Paxs	767.55	Joback Method

dvisc	0.0000909	Paxs	712.44	Joback Method
dvisc	0.0001244	Paxs	657.34	Joback Method
dvisc	0.0001802	Paxs	602.23	Joback Method
dvisc	0.0002814	Paxs	547.12	Joback Method
dvisc	0.0004856	Paxs	492.02	Joback Method
dvisc	0.0009615	Paxs	436.91	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=U405841&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405841&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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