

# Fumaric acid, 4-chlorobenzyl 3-chlorophenyl ester

Inchi:	InChI=1S/C17H12Cl2O4/c18-13-6-4-12(5-7-13)11-22-16(20)8-9-17(21)23-15-3-1-2-14(19)
InchiKey:	KZGJOLRIXGDDHS-CMDGGOBGSA-N
Formula:	C17H12Cl2O4
SMILES:	O=C(C=CC(=O)Oc1cccc(Cl)c1)OCc1ccc(Cl)cc1
Mol. weight [g/mol]:	351.18

## Physical Properties

Property code	Value	Unit	Source
gf	-113.66	kJ/mol	Joback Method
hf	-347.95	kJ/mol	Joback Method
hfus	41.26	kJ/mol	Joback Method
hvap	86.35	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.198		Crippen Method
mcvol	237.930	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinpola	2658.00		NIST Webbook
rinpola	2658.00		NIST Webbook
tb	883.28	K	Joback Method
tc	1128.36	K	Joback Method
tf	558.31	K	Joback Method
vc	0.897	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.22	J/molxK	883.28	Joback Method
cpg	637.70	J/molxK	924.13	Joback Method
cpg	647.06	J/molxK	964.97	Joback Method
cpg	655.36	J/molxK	1005.82	Joback Method
cpg	662.65	J/molxK	1046.66	Joback Method
cpg	668.99	J/molxK	1087.51	Joback Method
cpg	674.43	J/molxK	1128.36	Joback Method
dvisc	0.0003929	Paxs	558.31	Joback Method

dvisc	0.0002470	Paxs	612.47	Joback Method
dvisc	0.0001674	Paxs	666.63	Joback Method
dvisc	0.0001203	Paxs	720.80	Joback Method
dvisc	0.0000905	Paxs	774.96	Joback Method
dvisc	0.0000707	Paxs	829.12	Joback Method
dvisc	0.0000569	Paxs	883.28	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=U405922&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405922&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>
<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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