

# Fumaric acid, di(2,3,6-trichlorophenyl) ester

**Inchi:** InChI=1S/C16H6Cl6O4/c17-7-1-3-9(19)15(13(7)21)25-11(23)5-6-12(24)26-16-10(20)4-2  
**InchiKey:** LGRPINVRSGDPDU-AATRIKPKSA-N  
**Formula:** C16H6Cl6O4  
**SMILES:** O=C(C=CC(=O)Oc1c(Cl)ccc(Cl)c1Cl)Oc1c(Cl)ccc(Cl)c1Cl  
**Mol. weight [g/mol]:** 474.93

## Physical Properties

Property code	Value	Unit	Source
gf	-208.32	kJ/mol	Joback Method
hf	-436.15	kJ/mol	Joback Method
hfus	53.90	kJ/mol	Joback Method
hvap	104.31	kJ/mol	Joback Method
log10ws	-7.71		Crippen Method
logp	6.674		Crippen Method
mcvol	272.800	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
rinpol	3288.00		NIST Webbook
rinpol	3288.00		NIST Webbook
tb	1030.04	K	Joback Method
tc	1290.67	K	Joback Method
tf	716.80	K	Joback Method
vc	1.038	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.63	J/molxK	1030.04	Joback Method
cpg	632.60	J/molxK	1073.48	Joback Method
cpg	636.51	J/molxK	1116.92	Joback Method
cpg	639.40	J/molxK	1160.36	Joback Method
cpg	641.30	J/molxK	1203.79	Joback Method
cpg	642.23	J/molxK	1247.23	Joback Method
cpg	642.22	J/molxK	1290.67	Joback Method
dvisc	0.0001564	Paxs	716.80	Joback Method

dvisc	0.0001142	Paxs	769.01	Joback Method
dvisc	0.0000868	Paxs	821.21	Joback Method
dvisc	0.0000682	Paxs	873.42	Joback Method
dvisc	0.0000550	Paxs	925.63	Joback Method
dvisc	0.0000455	Paxs	977.83	Joback Method
dvisc	0.0000383	Paxs	1030.04	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=U348230&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348230&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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