

# Fumaric acid, 2,4-dichlorophenyl 3-methylbut-2-en-1-yl ester

<b>Inchi:</b>	InChI=1S/C15H14Cl2O4/c1-10(2)7-8-20-14(18)5-6-15(19)21-13-4-3-11(16)9-12(13)17/h3
<b>InchiKey:</b>	FVXYZDHFPOCYNB-AATRIKPKSA-N
<b>Formula:</b>	C15H14Cl2O4
<b>SMILES:</b>	CC(C)=CCOC(=O)C=CC(=O)Oc1ccc(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	329.18

## Physical Properties

Property code	Value	Unit	Source
gf	-171.24	kJ/mol	Joback Method
hf	-435.77	kJ/mol	Joback Method
hfus	40.93	kJ/mol	Joback Method
hvap	79.66	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	3.964		Crippen Method
mcvol	229.210	ml/mol	McGowan Method
pc	2010.90	kPa	Joback Method
rinpol	2283.00		NIST Webbook
rinpol	2283.00		NIST Webbook
tb	814.88	K	Joback Method
tc	1042.21	K	Joback Method
tf	490.31	K	Joback Method
vc	0.875	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.33	J/molxK	814.88	Joback Method
cpg	601.88	J/molxK	852.77	Joback Method
cpg	612.54	J/molxK	890.66	Joback Method
cpg	622.36	J/molxK	928.55	Joback Method
cpg	631.38	J/molxK	966.44	Joback Method
cpg	639.64	J/molxK	1004.32	Joback Method
cpg	647.18	J/molxK	1042.21	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=U405694&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405694&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>hvp:</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>rinp:</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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