

# Fumaric acid, isobutyl 2-methylpent-3-yl ester

<b>Inchi:</b>	InChI=1S/C14H24O4/c1-6-12(11(4)5)18-14(16)8-7-13(15)17-9-10(2)3/h7-8,10-12H,6,9H
<b>InchiKey:</b>	MUZZLMBDKAWMGH-BQYQJAHWSA-N
<b>Formula:</b>	C14H24O4
<b>SMILES:</b>	CCC(OC(=O)C=CC(=O)OCC(C)C)C(C)C
<b>Mol. weight [g/mol]:</b>	256.34

## Physical Properties

Property code	Value	Unit	Source
gf	-327.94	kJ/mol	Joback Method
hf	-720.51	kJ/mol	Joback Method
hfus	27.22	kJ/mol	Joback Method
hvap	63.86	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.720		Crippen Method
mcvol	218.700	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
rinqol	1619.00		NIST Webbook
tb	675.14	K	Joback Method
tc	864.61	K	Joback Method
tf	341.78	K	Joback Method
vc	0.830	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.55	J/molxK	675.14	Joback Method
cpg	617.48	J/molxK	706.72	Joback Method
cpg	632.58	J/molxK	738.30	Joback Method
cpg	646.87	J/molxK	769.88	Joback Method
cpg	660.36	J/molxK	801.46	Joback Method
cpg	673.06	J/molxK	833.03	Joback Method
cpg	684.98	J/molxK	864.61	Joback Method
dvisc	0.0028493	Paxs	341.78	Joback Method
dvisc	0.0010436	Paxs	397.34	Joback Method

dvisc	0.0004891	Paxs	452.90	Joback Method
dvisc	0.0002705	Paxs	508.46	Joback Method
dvisc	0.0001681	Paxs	564.02	Joback Method
dvisc	0.0001138	Paxs	619.58	Joback Method
dvisc	0.0000821	Paxs	675.14	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=U348760&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348760&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>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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