

# Fumaric acid, 3-hexyl isobutyl ester

<b>Inchi:</b>	InChI=1S/C14H24O4/c1-5-7-12(6-2)18-14(16)9-8-13(15)17-10-11(3)4/h8-9,11-12H,5-7,1
<b>InchiKey:</b>	WSNXHOZHEYWWMI-CMDGGGOBGSA-N
<b>Formula:</b>	C14H24O4
<b>SMILES:</b>	CCCC(CC)OC(=O)C=CC(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	256.34

## Physical Properties

Property code	Value	Unit	Source
gf	-325.50	kJ/mol	Joback Method
hf	-715.23	kJ/mol	Joback Method
hfus	30.75	kJ/mol	Joback Method
hvap	64.25	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.864		Crippen Method
mvol	218.700	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
rinpol	1644.00		NIST Webbook
rinpol	1644.00		NIST Webbook
tb	675.58	K	Joback Method
tc	862.18	K	Joback Method
tf	356.78	K	Joback Method
vc	0.836	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.07	J/molxK	675.58	Joback Method
cpg	616.74	J/molxK	706.68	Joback Method
cpg	631.60	J/molxK	737.78	Joback Method
cpg	645.68	J/molxK	768.88	Joback Method
cpg	658.99	J/molxK	799.98	Joback Method
cpg	671.55	J/molxK	831.08	Joback Method
cpg	683.37	J/molxK	862.18	Joback Method
dvisc	0.0021664	Paxs	356.78	Joback Method

dvisc	0.0009003	Paxs	409.91	Joback Method
dvisc	0.0004576	Paxs	463.05	Joback Method
dvisc	0.0002674	Paxs	516.18	Joback Method
dvisc	0.0001727	Paxs	569.31	Joback Method
dvisc	0.0001202	Paxs	622.45	Joback Method
dvisc	0.0000886	Paxs	675.58	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=U348603&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348603&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>

## 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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