

# Fumaric acid, 3-methylbutyl hex-4-yn-3-yl ester

Inchi:	InChI=1S/C15H22O4/c1-5-7-13(6-2)19-15(17)9-8-14(16)18-11-10-12(3)4/h8-9,12-13H,6,
InchiKey:	SONHRYHTAHHGHU-CMDGGOBGSA-N
Formula:	C15H22O4
SMILES:	CC#CC(CC)OC(=O)C=CC(=O)OCCC(C)C
Mol. weight [g/mol]:	266.33

## Physical Properties

Property code	Value	Unit	Source
gf	-114.28	kJ/mol	Joback Method
hf	-463.57	kJ/mol	Joback Method
hfus	36.46	kJ/mol	Joback Method
hvap	68.63	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	2.477		Crippen Method
mcvol	224.190	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
rinpol	1816.00		NIST Webbook
rinpol	1816.00		NIST Webbook
tb	707.46	K	Joback Method
tc	909.43	K	Joback Method
tf	474.15	K	Joback Method
vc	0.854	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.66	J/mol×K	707.46	Joback Method
cpg	626.20	J/mol×K	741.12	Joback Method
cpg	640.87	J/mol×K	774.78	Joback Method
cpg	654.68	J/mol×K	808.44	Joback Method
cpg	667.64	J/mol×K	842.10	Joback Method
cpg	679.78	J/mol×K	875.77	Joback Method
cpg	691.09	J/mol×K	909.43	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=U405549&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405549&amp;Units=SI</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>hvpap:</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>rinppl:</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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