

# Fumaric acid, 2-methylpentyl tridec-2-yn-1-yl ester

Inchi:	InChI=1S/C23H38O4/c1-4-6-7-8-9-10-11-12-13-14-15-19-26-22(24)17-18-23(25)27-20-2
InchiKey:	WEGGKZKCWIOURO-ISLYRVAYSA-N
Formula:	C23H38O4
SMILES:	CCCCCCCCCCC#CCOC(=O)C=CC(=O)OCC(C)CCC
Mol. weight [g/mol]:	378.55

## Physical Properties

Property code	Value	Unit	Source
gf	-44.48	kJ/mol	Joback Method
hf	-623.41	kJ/mol	Joback Method
hfus	60.70	kJ/mol	Joback Method
hvap	86.83	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	5.599		Crippen Method
mvol	336.910	ml/mol	McGowan Method
pc	1031.25	kPa	Joback Method
rinpol	2651.00		NIST Webbook
rinpol	2651.00		NIST Webbook
tb	890.94	K	Joback Method
tc	1092.76	K	Joback Method
tf	579.31	K	Joback Method
vc	1.308	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1076.00	J/molxK	890.94	Joback Method
cpg	1093.88	J/molxK	924.58	Joback Method
cpg	1110.60	J/molxK	958.21	Joback Method
cpg	1126.18	J/molxK	991.85	Joback Method
cpg	1140.67	J/molxK	1025.49	Joback Method
cpg	1154.10	J/molxK	1059.13	Joback Method
cpg	1166.50	J/molxK	1092.76	Joback Method

# Sources

<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=U405656&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405656&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# 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>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>rinpola:</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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