

# Fumaric acid, 4-octyl dodec-2-en-1-yl ester

<b>Inchi:</b>	InChI=1S/C24H42O4/c1-4-7-9-10-11-12-13-14-15-16-21-27-23(25)19-20-24(26)28-22(17
<b>InchiKey:</b>	XHJZDBINWGDWGA-LMOVRVBNSA-N
<b>Formula:</b>	C24H42O4
<b>SMILES:</b>	CCCCCCCCC=CCOC(=O)C=CC(=O)OC(CCC)CCCC
<b>Mol. weight [g/mol]:</b>	394.59

## Physical Properties

Property code	Value	Unit	Source
gf	-158.64	kJ/mol	Joback Method
hf	-799.13	kJ/mol	Joback Method
hfus	60.37	kJ/mol	Joback Method
hvap	86.86	kJ/mol	Joback Method
log10ws	-7.41		Crippen Method
logp	6.685		Crippen Method
mvol	355.300	ml/mol	McGowan Method
pc	908.34	kPa	Joback Method
rinpol	2651.00		NIST Webbook
rinpol	2651.00		NIST Webbook
tb	908.98	K	Joback Method
tc	1112.85	K	Joback Method
tf	479.40	K	Joback Method
vc	1.381	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1163.79	J/molxK	908.98	Joback Method
cpg	1182.74	J/molxK	942.96	Joback Method
cpg	1200.51	J/molxK	976.94	Joback Method
cpg	1217.15	J/molxK	1010.92	Joback Method
cpg	1232.73	J/molxK	1044.89	Joback Method
cpg	1247.29	J/molxK	1078.87	Joback Method
cpg	1260.91	J/molxK	1112.85	Joback Method
dvisc	0.0005301	Paxs	479.40	Joback Method

dvisc	0.0002169	Paxs	551.00	Joback Method
dvisc	0.0001090	Paxs	622.59	Joback Method
dvisc	0.0000631	Paxs	694.19	Joback Method
dvisc	0.0000405	Paxs	765.79	Joback Method
dvisc	0.0000280	Paxs	837.38	Joback Method
dvisc	0.0000205	Paxs	908.98	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=U405627&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405627&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>
<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>

## Legend

<b>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</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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