

# Fumaric acid, dec-4-enyl octyl ester

<b>Inchi:</b>	InChI=1S/C22H38O4/c1-3-5-7-9-11-12-14-16-20-26-22(24)18-17-21(23)25-19-15-13-10-
<b>InchiKey:</b>	VMLBRWXAHPJBIW-WCPGOBTASA-N
<b>Formula:</b>	C22H38O4
<b>SMILES:</b>	CCCCC=CCCCOC(=O)C=CC(=O)OCCCCCCCC
<b>Mol. weight [g/mol]:</b>	366.53

## Physical Properties

Property code	Value	Unit	Source
gf	-173.04	kJ/mol	Joback Method
hf	-752.57	kJ/mol	Joback Method
hfus	58.71	kJ/mol	Joback Method
hvap	82.79	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	5.906		Crippen Method
mvol	327.120	ml/mol	McGowan Method
pc	1018.13	kPa	Joback Method
rinpol	2570.00		NIST Webbook
rinpol	2570.00		NIST Webbook
tb	863.66	K	Joback Method
tc	1058.41	K	Joback Method
tf	471.86	K	Joback Method
vc	1.276	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1039.41	J/molxK	863.66	Joback Method
cpg	1119.40	J/molxK	1025.96	Joback Method
cpg	1105.31	J/molxK	993.50	Joback Method
cpg	1090.31	J/molxK	961.04	Joback Method
cpg	1074.36	J/molxK	928.58	Joback Method
cpg	1057.40	J/molxK	896.12	Joback Method
cpg	1132.62	J/molxK	1058.41	Joback Method
dvisc	0.0000302	Paxs	863.66	Joback Method

dvisc	0.0000405	Paxs	798.36	Joback Method
dvisc	0.0000570	Paxs	733.06	Joback Method
dvisc	0.0000858	Paxs	667.76	Joback Method
dvisc	0.0001413	Paxs	602.46	Joback Method
dvisc	0.0002626	Paxs	537.16	Joback Method
dvisc	0.0005794	Paxs	471.86	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=U348943&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348943&amp;Units=SI</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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