

# Fumaric acid, 2-methylpentyl octadecyl ester

**Inchi:** InChI=1S/C28H52O4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-24-31-27(29)22-2  
**InchiKey:** FKMJQVFLBWIQFB-GHVJWSGMSA-N  
**Formula:** C28H52O4  
**SMILES:** CCCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OCC(C)CCC  
**Mol. weight [g/mol]:** 452.71

## Physical Properties

Property code	Value	Unit	Source
gf	-205.18	kJ/mol	Joback Method
hf	-998.91	kJ/mol	Joback Method
hfus	70.53	kJ/mol	Joback Method
hvap	95.80	kJ/mol	Joback Method
log10ws	-8.88		Crippen Method
logp	8.327		Crippen Method
mcvol	415.960	ml/mol	McGowan Method
pc	709.60	kPa	Joback Method
rinpol	3077.00		NIST Webbook
rinpol	3077.00		NIST Webbook
tb	996.34	K	Joback Method
tc	1231.91	K	Joback Method
tf	529.56	K	Joback Method
vc	1.625	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1446.75	J/molxK	996.34	Joback Method
cpg	1468.66	J/molxK	1035.60	Joback Method
cpg	1488.79	J/molxK	1074.86	Joback Method
cpg	1507.22	J/molxK	1114.12	Joback Method
cpg	1524.05	J/molxK	1153.39	Joback Method
cpg	1539.36	J/molxK	1192.65	Joback Method
cpg	1553.25	J/molxK	1231.91	Joback Method
dvisc	0.0003320	Paxs	529.56	Joback Method

dvisc	0.0001357	Paxs	607.36	Joback Method
dvisc	0.0000680	Paxs	685.15	Joback Method
dvisc	0.0000392	Paxs	762.95	Joback Method
dvisc	0.0000250	Paxs	840.75	Joback Method
dvisc	0.0000173	Paxs	918.54	Joback Method
dvisc	0.0000126	Paxs	996.34	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=U348736&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348736&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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