

# Fumaric acid, di(4-heptyl) ester

**Inchi:** InChI=1S/C18H32O4/c1-5-9-15(10-6-2)21-17(19)13-14-18(20)22-16(11-7-3)12-8-4/h13-14  
**InchiKey:** NNJNXZGVWDWFTC-BUHFOSPRSA-N  
**Formula:** C18H32O4  
**SMILES:** CCCC(CCC)OC(=O)C=CC(=O)OC(CCC)CCC  
**Mol. weight [g/mol]:** 312.44

## Physical Properties

Property code	Value	Unit	Source
gf	-291.82	kJ/mol	Joback Method
hf	-797.79	kJ/mol	Joback Method
hfus	41.11	kJ/mol	Joback Method
hvap	73.16	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.567		Crippen Method
mcvol	275.060	ml/mol	McGowan Method
pc	1288.36	kPa	Joback Method
rinpol	1969.00		NIST Webbook
rinpol	1969.00		NIST Webbook
tb	767.10	K	Joback Method
tc	952.42	K	Joback Method
tf	401.86	K	Joback Method
vc	1.060	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.20	J/molxK	767.10	Joback Method
cpg	843.39	J/molxK	797.99	Joback Method
cpg	859.63	J/molxK	828.87	Joback Method
cpg	874.95	J/molxK	859.76	Joback Method
cpg	889.37	J/molxK	890.65	Joback Method
cpg	902.91	J/molxK	921.53	Joback Method
cpg	915.59	J/molxK	952.42	Joback Method
dvisc	0.0014223	Paxs	401.86	Joback Method

dvisc	0.0005699	Paxs	462.73	Joback Method
dvisc	0.0002825	Paxs	523.61	Joback Method
dvisc	0.0001620	Paxs	584.48	Joback Method
dvisc	0.0001032	Paxs	645.35	Joback Method
dvisc	0.0000711	Paxs	706.23	Joback Method
dvisc	0.0000519	Paxs	767.10	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=U348526&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348526&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.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>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>h<sub>vap</sub>:</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>log<sub>p</sub>:</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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