

# Fumaric acid, 3-heptyl pentyl ester

<b>Inchi:</b>	InChI=1S/C16H28O4/c1-4-7-9-13-19-15(17)11-12-16(18)20-14(6-3)10-8-5-2/h11-12,14H
<b>InchiKey:</b>	ABHBZUUFIKVBKY-VAWYXSNFSA-N
<b>Formula:</b>	C16H28O4
<b>SMILES:</b>	CCCCCOC(=O)C=CC(=O)OC(CC)CCCC
<b>Mol. weight [g/mol]:</b>	284.39

## Physical Properties

Property code	Value	Unit	Source
gf	-306.22	kJ/mol	Joback Method
hf	-751.23	kJ/mol	Joback Method
hfus	39.45	kJ/mol	Joback Method
hvap	69.09	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.788		Crippen Method
mcvol	246.880	ml/mol	McGowan Method
pc	1477.02	kPa	Joback Method
rinpol	1881.00		NIST Webbook
rinpol	1881.00		NIST Webbook
tb	721.78	K	Joback Method
tc	904.51	K	Joback Method
tf	394.32	K	Joback Method
vc	0.954	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.90	J/molxK	721.78	Joback Method
cpg	727.17	J/molxK	752.23	Joback Method
cpg	742.59	J/molxK	782.69	Joback Method
cpg	757.19	J/molxK	813.14	Joback Method
cpg	770.99	J/molxK	843.60	Joback Method
cpg	783.99	J/molxK	874.05	Joback Method
cpg	796.23	J/molxK	904.51	Joback Method
dvisc	0.0014186	Paxs	394.32	Joback Method

dvisc	0.0006427	Paxs	448.90	Joback Method
dvisc	0.0003457	Paxs	503.47	Joback Method
dvisc	0.0002100	Paxs	558.05	Joback Method
dvisc	0.0001394	Paxs	612.63	Joback Method
dvisc	0.0000989	Paxs	667.20	Joback Method
dvisc	0.0000739	Paxs	721.78	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=U348681&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348681&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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