

# Fumaric acid, 4-heptyl nonyl ester

<b>Inchi:</b>	InChI=1S/C20H36O4/c1-4-7-8-9-10-11-12-17-23-19(21)15-16-20(22)24-18(13-5-2)14-6-3
<b>InchiKey:</b>	BKSFAPILEUMUNB-FOCLMDBBSA-N
<b>Formula:</b>	C20H36O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)C=CC(=O)OC(CCC)CCC
<b>Mol. weight [g/mol]:</b>	340.50

## Physical Properties

Property code	Value	Unit	Source
gf	-272.54	kJ/mol	Joback Method
hf	-833.79	kJ/mol	Joback Method
hfus	49.81	kJ/mol	Joback Method
hvap	78.00	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	5.348		Crippen Method
mcvol	303.240	ml/mol	McGowan Method
pc	1121.55	kPa	Joback Method
rinsol	2268.00		NIST Webbook
tb	813.30	K	Joback Method
tc	1000.35	K	Joback Method
tf	439.40	K	Joback Method
vc	1.177	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	944.36	J/molxK	813.30	Joback Method
cpg	1023.32	J/molxK	969.18	Joback Method
cpg	1009.45	J/molxK	938.00	Joback Method
cpg	994.65	J/molxK	906.83	Joback Method
cpg	978.88	J/molxK	875.65	Joback Method
cpg	962.12	J/molxK	844.48	Joback Method
cpg	1036.28	J/molxK	1000.35	Joback Method
dvisc	0.0000425	Paxs	813.30	Joback Method
dvisc	0.0000574	Paxs	750.98	Joback Method

dvisc	0.0000819	Paxs	688.67	Joback Method
dvisc	0.0001253	Paxs	626.35	Joback Method
dvisc	0.0002106	Paxs	564.03	Joback Method
dvisc	0.0004027	Paxs	501.72	Joback Method
dvisc	0.0009257	Paxs	439.40	Joback Method

## Sources

<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=U348519&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348519&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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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