

# Fumaric acid, decyl 4-methylpent-2-yl ester

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

## Physical Properties

Property code	Value	Unit	Source
gf	-274.98	kJ/mol	Joback Method
hf	-839.07	kJ/mol	Joback Method
hfus	46.29	kJ/mol	Joback Method
hvap	77.61	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	5.204		Crippen Method
mcvol	303.240	ml/mol	McGowan Method
pc	1127.59	kPa	Joback Method
rinpol	2249.00		NIST Webbook
rinpol	2249.00		NIST Webbook
tb	812.86	K	Joback Method
tc	1000.99	K	Joback Method
tf	424.40	K	Joback Method
vc	1.171	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	944.85	J/molxK	812.86	Joback Method
cpg	1024.11	J/molxK	969.63	Joback Method
cpg	1010.22	J/molxK	938.28	Joback Method
cpg	995.38	J/molxK	906.92	Joback Method
cpg	979.55	J/molxK	875.57	Joback Method
cpg	962.71	J/molxK	844.21	Joback Method
cpg	1037.07	J/molxK	1000.99	Joback Method
dvisc	0.0000390	Paxs	812.86	Joback Method

dvisc	0.0000536	Paxs	748.12	Joback Method
dvisc	0.0000782	Paxs	683.37	Joback Method
dvisc	0.0001235	Paxs	618.63	Joback Method
dvisc	0.0002170	Paxs	553.89	Joback Method
dvisc	0.0004425	Paxs	489.14	Joback Method
dvisc	0.0011216	Paxs	424.40	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U348324&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348324&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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