

# Fumaric acid, 10-chlorodecyl nonyl ester

<b>Inchi:</b>	InChI=1S/C23H41ClO4/c1-2-3-4-5-9-12-15-20-27-22(25)17-18-23(26)28-21-16-13-10-7-6
<b>InchiKey:</b>	ACJORMVAPZCSEZ-ISLYRVAYSA-N
<b>Formula:</b>	C23H41ClO4
<b>SMILES:</b>	CCCCCCCCCOC(=O)C=CC(=O)OCCCCCCCCCCI
<b>Mol. weight [g/mol]:</b>	417.02

## Physical Properties

Property code	Value	Unit	Source
gf	-256.77	kJ/mol	Joback Method
hf	-906.17	kJ/mol	Joback Method
hfus	65.30	kJ/mol	Joback Method
hvap	89.45	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	6.739		Crippen Method
mvol	357.750	ml/mol	McGowan Method
pc	907.79	kPa	Joback Method
rinpol	3015.00		NIST Webbook
rinpol	3015.00		NIST Webbook
tb	919.81	K	Joback Method
tc	1126.54	K	Joback Method
tf	518.13	K	Joback Method
vc	1.401	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1158.26	J/molxK	919.81	Joback Method
cpg	1176.44	J/molxK	954.26	Joback Method
cpg	1193.37	J/molxK	988.72	Joback Method
cpg	1209.10	J/molxK	1023.17	Joback Method
cpg	1223.68	J/molxK	1057.63	Joback Method
cpg	1237.16	J/molxK	1092.08	Joback Method
cpg	1249.57	J/molxK	1126.54	Joback Method
dvisc	0.0004288	Paxs	518.13	Joback Method

dvisc	0.0002042	Paxs	585.08	Joback Method
dvisc	0.0001132	Paxs	652.02	Joback Method
dvisc	0.0000701	Paxs	718.97	Joback Method
dvisc	0.0000471	Paxs	785.92	Joback Method
dvisc	0.0000336	Paxs	852.86	Joback Method
dvisc	0.0000253	Paxs	919.81	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U348313&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348313&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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