

# Succinic acid, (5-ethyl-1,3-dioxan-5-yl)methyl nonyl ester

<b>Inchi:</b>	InChI=1S/C20H36O6/c1-3-5-6-7-8-9-10-13-25-18(21)11-12-19(22)26-16-20(4-2)14-23-17
<b>InchiKey:</b>	AGUYTFOHZDCLFN-UHFFFAOYSA-N
<b>Formula:</b>	C20H36O6
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCC(=O)OCC1(CC)COCOC1
<b>Mol. weight [g/mol]:</b>	372.50

## Physical Properties

Property code	Value	Unit	Source
gf	-503.60	kJ/mol	Joback Method
hf	-1140.17	kJ/mol	Joback Method
hfus	54.62	kJ/mol	Joback Method
hvap	86.72	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	4.004		Crippen Method
mvol	308.420	ml/mol	McGowan Method
pc	1262.85	kPa	Joback Method
rinpol	2586.00		NIST Webbook
rinpol	2586.00		NIST Webbook
tb	883.27	K	Joback Method
tc	1086.84	K	Joback Method
tf	543.90	K	Joback Method
vc	1.177	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1033.72	J/mol×K	883.27	Joback Method
cpg	1053.14	J/mol×K	917.20	Joback Method
cpg	1071.83	J/mol×K	951.13	Joback Method
cpg	1089.87	J/mol×K	985.05	Joback Method
cpg	1107.35	J/mol×K	1018.98	Joback Method
cpg	1124.38	J/mol×K	1052.91	Joback Method
cpg	1141.03	J/mol×K	1086.84	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=U382211&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382211&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>
<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>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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 vap:</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>r in pol:</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

Latest version available from:

<https://www.chemeo.com/cid/87-737-8/Succinic-acid-5-ethyl-1-3-dioxan-5-yl-methyl-nonyl-ester.pdf>

Generated by Cheméo on 2024-04-29 07:33:30.679513146 +0000 UTC m=+16665259.600090459.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.