

# Succinic acid, tridec-2-yn-1-yl tetrahydrofurfuryl ester

Inchi:	InChI=1S/C22H36O5/c1-2-3-4-5-6-7-8-9-10-11-12-17-26-21(23)15-16-22(24)27-19-20-14
InchiKey:	QXYAPINBCKZTRJ-UHFFFAOYSA-N
Formula:	C22H36O5
SMILES:	CCCCCCCCC#CCOC(=O)CCC(=O)OCC1CCCO1
Mol. weight [g/mol]:	380.52

## Physical Properties

Property code	Value	Unit	Source
gf	-180.25	kJ/mol	Joback Method
hf	-786.23	kJ/mol	Joback Method
hfus	63.35	kJ/mol	Joback Method
hvap	89.80	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	4.566		Crippen Method
mcvol	322.130	ml/mol	McGowan Method
pc	1183.34	kPa	Joback Method
rinsol	3011.00		NIST Webbook
tb	906.57	K	Joback Method
tc	1114.34	K	Joback Method
tf	625.59	K	Joback Method
vc	1.240	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1067.17	J/molxK	906.57	Joback Method
cpg	1084.57	J/molxK	941.20	Joback Method
cpg	1100.63	J/molxK	975.83	Joback Method
cpg	1115.38	J/molxK	1010.46	Joback Method
cpg	1128.85	J/molxK	1045.09	Joback Method
cpg	1141.08	J/molxK	1079.72	Joback Method
cpg	1152.10	J/molxK	1114.34	Joback Method

# Sources

<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=U390729&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390729&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>hvac:</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>mccol:</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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