

# Succinic acid, dodecyl 2,4,4-trimethylpentyl ester

Inchi:	InChI=1S/C24H46O4/c1-6-7-8-9-10-11-12-13-14-15-18-27-22(25)16-17-23(26)28-20-21(
InchiKey:	XWANGRRJNHSYKK-UHFFFAOYSA-N
Formula:	C24H46O4
SMILES:	CCCCCCCCCCCCOC(=O)CCC(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	398.62

## Physical Properties

Property code	Value	Unit	Source
gf	-316.24	kJ/mol	Joback Method
hf	-1042.32	kJ/mol	Joback Method
hfus	52.55	kJ/mol	Joback Method
hvap	85.65	kJ/mol	Joback Method
log10ws	-7.11		Crippen Method
logp	6.846		Crippen Method
mcvol	363.900	ml/mol	McGowan Method
pc	863.53	kPa	Joback Method
rinpol	2606.00		NIST Webbook
rinpol	2606.00		NIST Webbook
tb	897.43	K	Joback Method
tc	1098.73	K	Joback Method
tf	491.98	K	Joback Method
vc	1.411	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1218.06	J/molxK	897.43	Joback Method
cpg	1237.89	J/molxK	930.98	Joback Method
cpg	1256.38	J/molxK	964.53	Joback Method
cpg	1273.61	J/molxK	998.08	Joback Method
cpg	1289.60	J/molxK	1031.63	Joback Method
cpg	1304.43	J/molxK	1065.18	Joback Method
cpg	1318.12	J/molxK	1098.73	Joback Method
dvisc	0.0005616	Paxs	491.98	Joback Method

dvisc	0.0002329	Paxs	559.56	Joback Method
dvisc	0.0001168	Paxs	627.13	Joback Method
dvisc	0.0000670	Paxs	694.71	Joback Method
dvisc	0.0000424	Paxs	762.28	Joback Method
dvisc	0.0000289	Paxs	829.86	Joback Method
dvisc	0.0000209	Paxs	897.43	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=U381328&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381328&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>

## 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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