

# Succinic acid, 3-hexyl isobutyl ester

<b>Inchi:</b>	InChI=1S/C14H26O4/c1-5-7-12(6-2)18-14(16)9-8-13(15)17-10-11(3)4/h11-12H,5-10H2,1
<b>InchiKey:</b>	BWRRUPLQLPOKIK-UHFFFAOYSA-N
<b>Formula:</b>	C14H26O4
<b>SMILES:</b>	CCCC(CC)OC(=O)CCC(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	258.35

## Physical Properties

Property code	Value	Unit	Source
gf	-405.72	kJ/mol	Joback Method
hf	-832.45	kJ/mol	Joback Method
hfus	30.54	kJ/mol	Joback Method
hvap	64.29	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	3.088		Crippen Method
mcvol	223.000	ml/mol	McGowan Method
pc	1660.55	kPa	Joback Method
rinpol	1611.00		NIST Webbook
rinpol	1611.00		NIST Webbook
tb	671.42	K	Joback Method
tc	852.27	K	Joback Method
tf	361.86	K	Joback Method
vc	0.856	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.10	J/molxK	671.42	Joback Method
cpg	639.24	J/molxK	701.56	Joback Method
cpg	654.60	J/molxK	731.70	Joback Method
cpg	669.19	J/molxK	761.84	Joback Method
cpg	683.00	J/molxK	791.99	Joback Method
cpg	696.05	J/molxK	822.13	Joback Method
cpg	708.34	J/molxK	852.27	Joback Method
dvisc	0.0023105	Paxs	361.86	Joback Method

dvisc	0.0009958	Paxs	413.45	Joback Method
dvisc	0.0005173	Paxs	465.05	Joback Method
dvisc	0.0003062	Paxs	516.64	Joback Method
dvisc	0.0001994	Paxs	568.23	Joback Method
dvisc	0.0001395	Paxs	619.83	Joback Method
dvisc	0.0001031	Paxs	671.42	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U349442&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U349442&amp;Units=SI</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

Latest version available from:

<https://www.chemeo.com/cid/89-970-7/Succinic-acid-3-hexyl-isobutyl-ester.pdf>

Generated by Cheméo on 2024-04-28 21:27:24.735467942 +0000 UTC m=+16628893.656045253.

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