

# Succinic acid, 3-methylbenzyl propyl ester

<b>Inchi:</b>	InChI=1S/C15H20O4/c1-3-9-18-14(16)7-8-15(17)19-11-13-6-4-5-12(2)10-13/h4-6,10H,3,
<b>InchiKey:</b>	PPQBZHCNLSORKS-UHFFFAOYSA-N
<b>Formula:</b>	C15H20O4
<b>SMILES:</b>	CCCOC(=O)CCC(=O)OCc1cccc(C)c1
<b>Mol. weight [g/mol]:</b>	264.32

## Physical Properties

Property code	Value	Unit	Source
gf	-289.64	kJ/mol	Joback Method
hf	-617.47	kJ/mol	Joback Method
hfus	33.83	kJ/mol	Joback Method
hvap	70.23	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	2.772		Crippen Method
mvol	213.330	ml/mol	McGowan Method
pc	1975.31	kPa	Joback Method
rinpol	1932.00		NIST Webbook
rinpol	1932.00		NIST Webbook
tb	726.84	K	Joback Method
tc	930.46	K	Joback Method
tf	442.07	K	Joback Method
vc	0.816	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.63	J/molxK	726.84	Joback Method
cpg	608.41	J/molxK	760.78	Joback Method
cpg	622.26	J/molxK	794.71	Joback Method
cpg	635.18	J/molxK	828.65	Joback Method
cpg	647.19	J/molxK	862.59	Joback Method
cpg	658.30	J/molxK	896.52	Joback Method
cpg	668.51	J/molxK	930.46	Joback Method
dvisc	0.0009203	Paxs	442.07	Joback Method

dvisc	0.0005387	Paxs	489.53	Joback Method
dvisc	0.0003467	Paxs	536.99	Joback Method
dvisc	0.0002396	Paxs	584.46	Joback Method
dvisc	0.0001751	Paxs	631.92	Joback Method
dvisc	0.0001337	Paxs	679.38	Joback Method
dvisc	0.0001057	Paxs	726.84	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=U382389&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382389&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>

## 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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