

# Succinic acid, 3-chlorobenzyl isobutyl ester

<b>Inchi:</b>	InChI=1S/C15H19ClO4/c1-11(2)9-19-14(17)6-7-15(18)20-10-12-4-3-5-13(16)8-12/h3-5,8
<b>InchiKey:</b>	NTXZMKLDPLZRSY-UHFFFAOYSA-N
<b>Formula:</b>	C15H19ClO4
<b>SMILES:</b>	CC(C)COC(=O)CCC(=O)OCc1cccc(Cl)c1
<b>Mol. weight [g/mol]:</b>	298.76

## Physical Properties

Property code	Value	Unit	Source
gf	-304.01	kJ/mol	Joback Method
hf	-638.49	kJ/mol	Joback Method
hfus	34.51	kJ/mol	Joback Method
hvap	74.23	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.363		Crippen Method
mcvol	225.570	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
rinsol	2080.00		NIST Webbook
tb	763.83	K	Joback Method
tc	974.13	K	Joback Method
tf	456.99	K	Joback Method
vc	0.859	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.63	J/molxK	763.83	Joback Method
cpg	634.52	J/molxK	798.88	Joback Method
cpg	647.43	J/molxK	833.93	Joback Method
cpg	659.36	J/molxK	868.98	Joback Method
cpg	670.31	J/molxK	904.03	Joback Method
cpg	680.32	J/molxK	939.08	Joback Method
cpg	689.38	J/molxK	974.13	Joback Method
dvisc	0.0008947	Paxs	456.99	Joback Method
dvisc	0.0004991	Paxs	508.13	Joback Method

dvisc	0.0003097	Paxs	559.27	Joback Method
dvisc	0.0002082	Paxs	610.41	Joback Method
dvisc	0.0001489	Paxs	661.55	Joback Method
dvisc	0.0001117	Paxs	712.69	Joback Method
dvisc	0.0000870	Paxs	763.83	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U381699&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381699&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>
<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>

## 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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