

# Succinic acid, ethyl 2-iodobenzyl ester

**Inchi:** InChI=1S/C13H15IO4/c1-2-17-12(15)7-8-13(16)18-9-10-5-3-4-6-11(10)14/h3-6H,2,7-9H2  
**InchiKey:** MHDQPTXYCXZCGB-UHFFFAOYSA-N  
**Formula:** C13H15IO4  
**SMILES:** CCOC(=O)CCC(=O)OCc1ccccc1I  
**Mol. weight [g/mol]:** 362.16

## Physical Properties

Property code	Value	Unit	Source
gf	-248.36	kJ/mol	Joback Method
hf	-499.32	kJ/mol	Joback Method
hfus	33.06	kJ/mol	Joback Method
hvap	75.16	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	2.678		Crippen Method
mvol	210.970	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
rinpol	2137.00		NIST Webbook
rinpol	2137.00		NIST Webbook
tb	774.22	K	Joback Method
tc	1004.72	K	Joback Method
tf	477.59	K	Joback Method
vc	0.791	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.49	J/molxK	774.22	Joback Method
cpg	586.01	J/molxK	966.31	Joback Method
cpg	577.59	J/molxK	927.89	Joback Method
cpg	568.25	J/molxK	889.47	Joback Method
cpg	557.97	J/molxK	851.05	Joback Method
cpg	546.72	J/molxK	812.64	Joback Method
cpg	593.53	J/molxK	1004.72	Joback Method
dvisc	0.0001078	Paxs	774.22	Joback Method

dvisc	0.0001356	Paxs	724.78	Joback Method
dvisc	0.0001765	Paxs	675.34	Joback Method
dvisc	0.0002395	Paxs	625.90	Joback Method
dvisc	0.0003424	Paxs	576.47	Joback Method
dvisc	0.0005234	Paxs	527.03	Joback Method
dvisc	0.0008737	Paxs	477.59	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=U381099&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381099&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

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