

# Succinic acid, 3-iodobenzyl 2-methylhex-3-yl ester

Inchi:	InChI=1S/C18H25IO4/c1-4-6-16(13(2)3)23-18(21)10-9-17(20)22-12-14-7-5-8-15(19)11-1
InchiKey:	RJAZZWWYQOICNU-UHFFFAOYSA-N
Formula:	C18H25IO4
SMILES:	CCCC(OC(=O)CCC(=O)OCc1cccc(I)c1)C(C)C
Mol. weight [g/mol]:	432.29

## Physical Properties

Property code	Value	Unit	Source
gf	-211.14	kJ/mol	Joback Method
hf	-613.08	kJ/mol	Joback Method
hfus	38.96	kJ/mol	Joback Method
hvap	85.51	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	4.483		Crippen Method
mvol	281.420	ml/mol	McGowan Method
pc	1545.13	kPa	Joback Method
rinpol	2503.00		NIST Webbook
rinpol	2503.00		NIST Webbook
tb	887.74	K	Joback Method
tc	1111.68	K	Joback Method
tf	503.94	K	Joback Method
vc	1.060	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.61	J/molxK	887.74	Joback Method
cpg	827.46	J/molxK	925.06	Joback Method
cpg	840.11	J/molxK	962.39	Joback Method
cpg	851.60	J/molxK	999.71	Joback Method
cpg	861.97	J/molxK	1037.04	Joback Method
cpg	871.24	J/molxK	1074.36	Joback Method
cpg	879.47	J/molxK	1111.68	Joback Method
dvisc	0.0006556	Paxs	503.94	Joback Method

dvisc	0.0003239	Paxs	567.91	Joback Method
dvisc	0.0001845	Paxs	631.87	Joback Method
dvisc	0.0001166	Paxs	695.84	Joback Method
dvisc	0.0000796	Paxs	759.81	Joback Method
dvisc	0.0000577	Paxs	823.77	Joback Method
dvisc	0.0000438	Paxs	887.74	Joback Method

## Sources

<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=U381385&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381385&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>

## Legend

<b>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>c</sub>vol:</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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