

# Sebacic acid, 4-iodobenzyl propyl ester

<b>Inchi:</b>	InChI=1S/C20H29IO4/c1-2-15-24-19(22)9-7-5-3-4-6-8-10-20(23)25-16-17-11-13-18(21)1
<b>InchiKey:</b>	XJBNKSRNLFWHCD-UHFFFAOYSA-N
<b>Formula:</b>	C20H29IO4
<b>SMILES:</b>	CCCOC(=O)CCCCCCCCC(=O)OCc1ccc(I)cc1
<b>Mol. weight [g/mol]:</b>	460.35

## Physical Properties

Property code	Value	Unit	Source
gf	-189.42	kJ/mol	Joback Method
hf	-643.80	kJ/mol	Joback Method
hfus	51.19	kJ/mol	Joback Method
hvap	90.74	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	5.408		Crippen Method
mvol	309.600	ml/mol	McGowan Method
pc	1320.39	kPa	Joback Method
rinpol	2910.00		NIST Webbook
rinpol	2910.00		NIST Webbook
tb	934.38	K	Joback Method
tc	1153.60	K	Joback Method
tf	556.48	K	Joback Method
vc	1.183	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	929.57	J/molxK	934.38	Joback Method
cpg	943.53	J/molxK	970.92	Joback Method
cpg	956.30	J/molxK	1007.45	Joback Method
cpg	967.93	J/molxK	1043.99	Joback Method
cpg	978.46	J/molxK	1080.53	Joback Method
cpg	987.92	J/molxK	1117.07	Joback Method
cpg	996.37	J/molxK	1153.60	Joback Method
dvisc	0.0004156	Paxs	556.48	Joback Method

dvisc	0.0002288	Paxs	619.46	Joback Method
dvisc	0.0001406	Paxs	682.45	Joback Method
dvisc	0.0000938	Paxs	745.43	Joback Method
dvisc	0.0000667	Paxs	808.41	Joback Method
dvisc	0.0000498	Paxs	871.40	Joback Method
dvisc	0.0000387	Paxs	934.38	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=U380623&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380623&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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