

# Sebacic acid, ethyl 4-iodobenzyl ester

<b>Inchi:</b>	InChI=1S/C19H27IO4/c1-2-23-18(21)9-7-5-3-4-6-8-10-19(22)24-15-16-11-13-17(20)14-1
<b>InchiKey:</b>	BOTQKKPOOVEGPS-UHFFFAOYSA-N
<b>Formula:</b>	C19H27IO4
<b>SMILES:</b>	CCOC(=O)CCCCCCCC(=O)OCc1ccc(I)cc1
<b>Mol. weight [g/mol]:</b>	446.32

## Physical Properties

Property code	Value	Unit	Source
gf	-197.84	kJ/mol	Joback Method
hf	-623.16	kJ/mol	Joback Method
hfus	48.60	kJ/mol	Joback Method
hvap	88.51	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	5.018		Crippen Method
mvol	295.510	ml/mol	McGowan Method
pc	1417.57	kPa	Joback Method
rmpol	2812.00		NIST Webbook
rmpol	2812.00		NIST Webbook
tb	911.50	K	Joback Method
tc	1130.22	K	Joback Method
tf	545.21	K	Joback Method
vc	1.127	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	870.71	J/molxK	911.50	Joback Method
cpg	884.50	J/molxK	947.95	Joback Method
cpg	897.14	J/molxK	984.41	Joback Method
cpg	908.66	J/molxK	1020.86	Joback Method
cpg	919.11	J/molxK	1057.31	Joback Method
cpg	928.52	J/molxK	1093.76	Joback Method
cpg	936.92	J/molxK	1130.22	Joback Method
dvisc	0.0004671	Paxs	545.21	Joback Method

dvisc	0.0002599	Paxs	606.26	Joback Method
dvisc	0.0001610	Paxs	667.31	Joback Method
dvisc	0.0001081	Paxs	728.36	Joback Method
dvisc	0.0000772	Paxs	789.40	Joback Method
dvisc	0.0000578	Paxs	850.45	Joback Method
dvisc	0.0000450	Paxs	911.50	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=U380622&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380622&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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