

# Sebacic acid, (1,3-benzodioxol-5-yl)methyl hexyl ester

<b>Inchi:</b>	InChI=1S/C24H36O6/c1-2-3-4-11-16-27-23(25)12-9-7-5-6-8-10-13-24(26)28-18-20-14-15
<b>InchiKey:</b>	ZHYHWBQBWBUCX-UHFFFAOYSA-N
<b>Formula:</b>	C24H36O6
<b>SMILES:</b>	CCCCCOC(=O)CCCCCCCC(=O)OCc1ccc2c(c1)OCO2
<b>Mol. weight [g/mol]:</b>	420.54

## Physical Properties

Property code	Value	Unit	Source
gf	-327.27	kJ/mol	Joback Method
hf	-985.56	kJ/mol	Joback Method
hfus	69.77	kJ/mol	Joback Method
hvap	100.17	kJ/mol	Joback Method
log10ws	-6.98		Crippen Method
logp	5.703		Crippen Method
mvol	341.020	ml/mol	McGowan Method
pc	1123.06	kPa	Joback Method
rinpol	3091.00		NIST Webbook
rinpol	3091.00		NIST Webbook
tb	1003.05	K	Joback Method
tc	1228.03	K	Joback Method
tf	631.34	K	Joback Method
vc	1.319	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1161.40	J/molxK	1003.05	Joback Method
cpg	1177.06	J/molxK	1040.55	Joback Method
cpg	1191.48	J/molxK	1078.04	Joback Method
cpg	1204.74	J/molxK	1115.54	Joback Method
cpg	1216.90	J/molxK	1153.03	Joback Method
cpg	1228.04	J/molxK	1190.53	Joback Method
cpg	1238.23	J/molxK	1228.03	Joback Method
dvisc	0.0004142	Paxs	631.34	Joback Method

dvisc	0.0002552	Paxs	693.29	Joback Method
dvisc	0.0001702	Paxs	755.24	Joback Method
dvisc	0.0001207	Paxs	817.19	Joback Method
dvisc	0.0000898	Paxs	879.15	Joback Method
dvisc	0.0000695	Paxs	941.10	Joback Method
dvisc	0.0000555	Paxs	1003.05	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U380690&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380690&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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