

# Sebacic acid, isohexyl pent-4-enyl ester

<b>Inchi:</b>	InChI=1S/C21H38O4/c1-4-5-12-17-24-20(22)15-10-8-6-7-9-11-16-21(23)25-18-13-14-19
<b>InchiKey:</b>	GDHUKBZWNJOMLD-UHFFFAOYSA-N
<b>Formula:</b>	C21H38O4
<b>SMILES:</b>	C=CCCCOC(=O)CCCCCCCCC(=O)OCCCC(C)C
<b>Mol. weight [g/mol]:</b>	354.52

## Physical Properties

Property code	Value	Unit	Source
gf	-256.50	kJ/mol	Joback Method
hf	-846.22	kJ/mol	Joback Method
hfus	50.92	kJ/mol	Joback Method
hvap	79.59	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	5.596		Crippen Method
mvol	317.330	ml/mol	McGowan Method
pc	1045.97	kPa	Joback Method
rinpol	2451.00		NIST Webbook
rinpol	2451.00		NIST Webbook
tb	828.70	K	Joback Method
tc	1016.50	K	Joback Method
tf	453.99	K	Joback Method
vc	1.234	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1003.27	J/molxK	828.70	Joback Method
cpg	1021.45	J/molxK	860.00	Joback Method
cpg	1038.55	J/molxK	891.30	Joback Method
cpg	1054.58	J/molxK	922.60	Joback Method
cpg	1069.57	J/molxK	953.90	Joback Method
cpg	1083.55	J/molxK	985.20	Joback Method
cpg	1096.52	J/molxK	1016.50	Joback Method
dvisc	0.0008941	Paxs	453.99	Joback Method

dvisc	0.0004024	Paxs	516.44	Joback Method
dvisc	0.0002152	Paxs	578.89	Joback Method
dvisc	0.0001300	Paxs	641.35	Joback Method
dvisc	0.0000859	Paxs	703.80	Joback Method
dvisc	0.0000607	Paxs	766.25	Joback Method
dvisc	0.0000452	Paxs	828.70	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U355412&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355412&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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