

# Sebacic acid, heptyl pentyl ester

<b>Inchi:</b>	InChI=1S/C22H42O4/c1-3-5-7-12-16-20-26-22(24)18-14-11-9-8-10-13-17-21(23)25-19-1
<b>InchiKey:</b>	UFFLGXDDHOFUNJ-UHFFFAOYSA-N
<b>Formula:</b>	C22H42O4
<b>SMILES:</b>	CCCCCCCOC(=O)CCCCCCCC(=O)OCCCCC
<b>Mol. weight [g/mol]:</b>	370.57

## Physical Properties

Property code	Value	Unit	Source
gf	-333.48	kJ/mol	Joback Method
hf	-987.01	kJ/mol	Joback Method
hfus	58.31	kJ/mol	Joback Method
hvap	82.88	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	6.354		Crippen Method
mcvol	335.720	ml/mol	McGowan Method
pc	953.78	kPa	Joback Method
rinpol	2626.00		NIST Webbook
tb	855.34	K	Joback Method
tc	1047.20	K	Joback Method
tf	482.02	K	Joback Method
vc	1.315	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1092.06	J/molxK	855.34	Joback Method
cpg	1176.14	J/molxK	1015.23	Joback Method
cpg	1161.63	J/molxK	983.25	Joback Method
cpg	1145.99	J/molxK	951.27	Joback Method
cpg	1129.19	J/molxK	919.29	Joback Method
cpg	1111.23	J/molxK	887.32	Joback Method
cpg	1189.55	J/molxK	1047.20	Joback Method
dvisc	0.0000397	Paxs	855.34	Joback Method
dvisc	0.0000529	Paxs	793.12	Joback Method

dvisc	0.0000739	Paxs	730.90	Joback Method
dvisc	0.0001100	Paxs	668.68	Joback Method
dvisc	0.0001775	Paxs	606.46	Joback Method
dvisc	0.0003195	Paxs	544.24	Joback Method
dvisc	0.0006693	Paxs	482.02	Joback Method

## Sources

<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=U354306&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354306&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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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