

# Sebacic acid, heptyl 3-oxobut-2-yl ester

<b>Inchi:</b>	InChI=1S/C21H38O5/c1-4-5-6-11-14-17-25-20(23)15-12-9-7-8-10-13-16-21(24)26-19(3)
<b>InchiKey:</b>	LYWQLLWHSSBRKV-UHFFFAOYSA-N
<b>Formula:</b>	C21H38O5
<b>SMILES:</b>	CCCCCCCOC(=O)CCCCCCCC(=O)OC(C)C(C)=O
<b>Mol. weight [g/mol]:</b>	370.52

## Physical Properties

Property code	Value	Unit	Source
gf	-473.26	kJ/mol	Joback Method
hf	-1084.23	kJ/mol	Joback Method
hfus	53.80	kJ/mol	Joback Method
hvap	87.01	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	5.141		Crippen Method
mvol	323.200	ml/mol	McGowan Method
pc	1060.33	kPa	Joback Method
rinpol	2558.00		NIST Webbook
rinpol	2558.00		NIST Webbook
tb	885.89	K	Joback Method
tc	1084.76	K	Joback Method
tf	505.68	K	Joback Method
vc	1.260	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1053.22	J/molxK	885.89	Joback Method
cpg	1127.14	J/molxK	1051.61	Joback Method
cpg	1114.75	J/molxK	1018.47	Joback Method
cpg	1101.18	J/molxK	985.32	Joback Method
cpg	1086.42	J/molxK	952.18	Joback Method
cpg	1070.44	J/molxK	919.03	Joback Method
cpg	1138.39	J/molxK	1084.76	Joback Method
dvisc	0.0000398	Paxs	885.89	Joback Method

dvisc	0.0000531	Paxs	822.52	Joback Method
dvisc	0.0000743	Paxs	759.15	Joback Method
dvisc	0.0001105	Paxs	695.78	Joback Method
dvisc	0.0001780	Paxs	632.42	Joback Method
dvisc	0.0003187	Paxs	569.05	Joback Method
dvisc	0.0006604	Paxs	505.68	Joback Method

## Sources

<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=U355779&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355779&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>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</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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