

# Sebacic acid, 4-heptyl isoheptyl ester

<b>Inchi:</b>	InChI=1S/C23H44O4/c1-5-14-21(15-6-2)27-23(25)18-12-10-8-7-9-11-17-22(24)26-19-13
<b>InchiKey:</b>	WCIJPINYQDQOMI-UHFFFAOYSA-N
<b>Formula:</b>	C23H44O4
<b>SMILES:</b>	CCCC(CCC)OC(=O)CCCCCCCC(=O)OCCCC(C)C
<b>Mol. weight [g/mol]:</b>	384.59

## Physical Properties

Property code	Value	Unit	Source
gf	-329.94	kJ/mol	Joback Method
hf	-1018.21	kJ/mol	Joback Method
hfus	53.85	kJ/mol	Joback Method
hvap	84.33	kJ/mol	Joback Method
log10ws	-7.05		Crippen Method
logp	6.599		Crippen Method
mcvol	349.810	ml/mol	McGowan Method
pc	908.34	kPa	Joback Method
rinpola	2520.00		NIST Webbook
tb	877.34	K	Joback Method
tc	1074.11	K	Joback Method
tf	463.29	K	Joback Method
vc	1.359	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1155.40	J/molxK	877.34	Joback Method
cpg	1240.52	J/molxK	1041.32	Joback Method
cpg	1226.01	J/molxK	1008.52	Joback Method
cpg	1210.26	J/molxK	975.73	Joback Method
cpg	1193.27	J/molxK	942.93	Joback Method
cpg	1174.99	J/molxK	910.14	Joback Method
cpg	1253.84	J/molxK	1074.11	Joback Method
dvisc	0.0000286	Paxs	877.34	Joback Method
dvisc	0.0000394	Paxs	808.33	Joback Method

dvisc	0.0000577	Paxs	739.32	Joback Method
dvisc	0.0000911	Paxs	670.32	Joback Method
dvisc	0.0001600	Paxs	601.31	Joback Method
dvisc	0.0003252	Paxs	532.30	Joback Method
dvisc	0.0008160	Paxs	463.29	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U355386&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355386&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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