

# Sebacic acid, 2,4-dimethylpent-3-yl pentadecyl ester

Inchi:	InChI=1S/C32H62O4/c1-6-7-8-9-10-11-12-13-14-15-18-21-24-27-35-30(33)25-22-19-16-
InchiKey:	IQDRZKWTALQNIE-UHFFFAOYSA-N
Formula:	C32H62O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]:	510.83

## Physical Properties

Property code	Value	Unit	Source
gf	-256.60	kJ/mol	Joback Method
hf	-1209.25	kJ/mol	Joback Method
hfus	73.64	kJ/mol	Joback Method
hvap	103.97	kJ/mol	Joback Method
log10ws	-10.57		Crippen Method
logp	9.965		Crippen Method
mcvol	476.620	ml/mol	McGowan Method
pc	573.98	kPa	Joback Method
rinsol	3437.00		NIST Webbook
tb	1082.82	K	Joback Method
tc	1370.02	K	Joback Method
tf	549.72	K	Joback Method
vc	1.857	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1737.08	J/molxK	1082.82	Joback Method
cpg	1832.09	J/molxK	1322.15	Joback Method
cpg	1818.43	J/molxK	1274.29	Joback Method
cpg	1802.25	J/molxK	1226.42	Joback Method
cpg	1783.41	J/molxK	1178.55	Joback Method
cpg	1761.73	J/molxK	1130.69	Joback Method
cpg	1843.40	J/molxK	1370.02	Joback Method
dvisc	0.0000062	Paxs	1082.82	Joback Method
dvisc	0.0000087	Paxs	993.97	Joback Method

dvisc	0.0000132	Paxs	905.12	Joback Method
dvisc	0.0000217	Paxs	816.27	Joback Method
dvisc	0.0000406	Paxs	727.42	Joback Method
dvisc	0.0000901	Paxs	638.57	Joback Method
dvisc	0.0002592	Paxs	549.72	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=U355437&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355437&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>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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