

# Sebacic acid, dodec-9-ynyl isoheptyl ester

**Inchi:** InChI=1S/C28H50O4/c1-4-5-6-7-8-9-10-13-16-19-24-31-27(29)22-17-14-11-12-15-18-23  
**InchiKey:** MWLRCNRAXYBVNH-UHFFFAOYSA-N  
**Formula:** C28H50O4  
**SMILES:** CCC#CCCCCCCCCOC(=O)CCCCCCCC(=O)OCCCC(C)C  
**Mol. weight [g/mol]:** 450.69

## Physical Properties

Property code	Value	Unit	Source
gf	-82.60	kJ/mol	Joback Method
hf	-843.83	kJ/mol	Joback Method
hfus	73.45	kJ/mol	Joback Method
hvap	98.00	kJ/mol	Joback Method
log10ws	-8.82		Crippen Method
logp	7.774		Crippen Method
mvol	411.660	ml/mol	McGowan Method
pc	752.26	kPa	Joback Method
rinpol	3189.00		NIST Webbook
rinpol	3189.00		NIST Webbook
tb	1001.18	K	Joback Method
tc	1232.66	K	Joback Method
tf	640.74	K	Joback Method
vc	1.607	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1418.98	J/molxK	1001.18	Joback Method
cpg	1439.36	J/molxK	1039.76	Joback Method
cpg	1457.92	J/molxK	1078.34	Joback Method
cpg	1474.71	J/molxK	1116.92	Joback Method
cpg	1489.80	J/molxK	1155.50	Joback Method
cpg	1503.25	J/molxK	1194.08	Joback Method
cpg	1515.12	J/molxK	1232.66	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U355792&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355792&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>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>hvp:</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>rinp:</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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