

# Sebacic acid, cis-non-3-enyl isoheptyl ester

<b>Inchi:</b>	InChI=1S/C25H46O4/c1-4-5-6-7-10-13-16-21-28-24(26)19-14-11-8-9-12-15-20-25(27)29
<b>InchiKey:</b>	XIJVFPKPYORUSU-RAXLEYEMSA-N
<b>Formula:</b>	C25H46O4
<b>SMILES:</b>	CCCCC=CCCOC(=O)CCCCCCCC(=O)OCCCC(C)C
<b>Mol. weight [g/mol]:</b>	410.63

## Physical Properties

Property code	Value	Unit	Source
gf	-230.44	kJ/mol	Joback Method
hf	-936.99	kJ/mol	Joback Method
hfus	62.76	kJ/mol	Joback Method
hvap	89.13	kJ/mol	Joback Method
log10ws	-7.62		Crippen Method
logp	7.156		Crippen Method
mcvol	373.690	ml/mol	McGowan Method
pc	832.42	kPa	Joback Method
rinpola	2818.00		NIST Webbook
tb	927.70	K	Joback Method
tc	1137.27	K	Joback Method
tf	495.75	K	Joback Method
vc	1.458	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1254.19	J/molxK	927.70	Joback Method
cpg	1340.92	J/molxK	1102.34	Joback Method
cpg	1326.14	J/molxK	1067.41	Joback Method
cpg	1310.14	J/molxK	1032.49	Joback Method
cpg	1292.84	J/molxK	997.56	Joback Method
cpg	1274.21	J/molxK	962.63	Joback Method
cpg	1354.51	J/molxK	1137.27	Joback Method
dvisc	0.0000202	Paxs	927.70	Joback Method
dvisc	0.0000275	Paxs	855.71	Joback Method

dvisc	0.0000396	Paxs	783.72	Joback Method
dvisc	0.0000616	Paxs	711.72	Joback Method
dvisc	0.0001057	Paxs	639.73	Joback Method
dvisc	0.0002080	Paxs	567.74	Joback Method
dvisc	0.0004981	Paxs	495.75	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U355923&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355923&amp;Units=SI</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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