

# Sebacic acid, 1-naphthyl octyl ester

<b>Inchi:</b>	InChI=1S/C28H40O4/c1-2-3-4-5-10-15-23-31-27(29)21-11-8-6-7-9-12-22-28(30)32-26-20
<b>InchiKey:</b>	RYQXLAWADRJGCT-UHFFFAOYSA-N
<b>Formula:</b>	C28H40O4
<b>SMILES:</b>	CCCCCCCCOC(=O)CCCCCCCC(=O)Oc1cccc2ccccc12
<b>Mol. weight [g/mol]:</b>	440.61

## Physical Properties

Property code	Value	Unit	Source
gf	-73.53	kJ/mol	Joback Method
hf	-694.72	kJ/mol	Joback Method
hfus	64.52	kJ/mol	Joback Method
hvap	100.81	kJ/mol	Joback Method
log10ws	-9.15		Crippen Method
logp	7.770		Crippen Method
mvol	377.040	ml/mol	McGowan Method
pc	945.00	kPa	Joback Method
rinpol	3591.00		NIST Webbook
rinpol	3591.00		NIST Webbook
tb	1043.26	K	Joback Method
tc	1278.22	K	Joback Method
tf	621.28	K	Joback Method
vc	1.466	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1286.64	J/molxK	1043.26	Joback Method
cpg	1303.26	J/molxK	1082.42	Joback Method
cpg	1318.52	J/molxK	1121.58	Joback Method
cpg	1332.52	J/molxK	1160.74	Joback Method
cpg	1345.35	J/molxK	1199.90	Joback Method
cpg	1357.12	J/molxK	1239.06	Joback Method
cpg	1367.92	J/molxK	1278.22	Joback Method
dvisc	0.0003202	Paxs	621.28	Joback Method

dvisc	0.0001845	Paxs	691.61	Joback Method
dvisc	0.0001177	Paxs	761.94	Joback Method
dvisc	0.0000810	Paxs	832.27	Joback Method
dvisc	0.0000591	Paxs	902.60	Joback Method
dvisc	0.0000451	Paxs	972.93	Joback Method
dvisc	0.0000357	Paxs	1043.26	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=U354811&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354811&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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