

# Sebacic acid, isohexyl 2-naphthyl ester

<b>Inchi:</b>	InChI=1S/C26H36O4/c1-21(2)12-11-19-29-25(27)15-7-5-3-4-6-8-16-26(28)30-24-18-17-2
<b>InchiKey:</b>	IHFYKWSHXJXHKT-UHFFFAOYSA-N
<b>Formula:</b>	C26H36O4
<b>SMILES:</b>	CC(C)CCCOC(=O)CCCCCCCC(=O)Oc1ccc2ccccc2c1
<b>Mol. weight [g/mol]:</b>	412.56

## Physical Properties

Property code	Value	Unit	Source
gf	-92.81	kJ/mol	Joback Method
hf	-658.72	kJ/mol	Joback Method
hfus	55.82	kJ/mol	Joback Method
hvap	95.97	kJ/mol	Joback Method
log10ws	-8.07		Crippen Method
logp	6.845		Crippen Method
mvol	348.860	ml/mol	McGowan Method
pc	1072.87	kPa	Joback Method
rinpol	3377.00		NIST Webbook
tb	997.06	K	Joback Method
tc	1221.29	K	Joback Method
tf	583.74	K	Joback Method
vc	1.347	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1162.62	J/molxK	997.06	Joback Method
cpg	1178.51	J/molxK	1034.43	Joback Method
cpg	1193.12	J/molxK	1071.80	Joback Method
cpg	1206.54	J/molxK	1109.17	Joback Method
cpg	1218.86	J/molxK	1146.54	Joback Method
cpg	1230.14	J/molxK	1183.91	Joback Method
cpg	1240.47	J/molxK	1221.29	Joback Method
dvisc	0.0004275	Paxs	583.74	Joback Method
dvisc	0.0002389	Paxs	652.63	Joback Method

dvisc	0.0001492	Paxs	721.51	Joback Method
dvisc	0.0001012	Paxs	790.40	Joback Method
dvisc	0.0000730	Paxs	859.29	Joback Method
dvisc	0.0000553	Paxs	928.17	Joback Method
dvisc	0.0000435	Paxs	997.06	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=U354839&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354839&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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