

# Sebacic acid, isohexyl 3-propylphenyl ester

**Inchi:** InChI=1S/C25H40O4/c1-4-14-22-16-11-12-17-23(22)29-25(27)19-10-8-6-5-7-9-18-24(26)  
**InchiKey:** SQVQHWRKLXBGDR-UHFFFAOYSA-N  
**Formula:** C25H40O4  
**SMILES:** CCCc1ccccc1OC(=O)CCCCCCCCC(=O)OCCCC(C)C  
**Mol. weight [g/mol]:** 404.58

## Physical Properties

Property code	Value	Unit	Source
gf	-207.88	kJ/mol	Joback Method
hf	-829.15	kJ/mol	Joback Method
hfus	56.21	kJ/mol	Joback Method
hvap	92.11	kJ/mol	Joback Method
log10ws	-7.49		Crippen Method
logp	6.645		Crippen Method
mvol	354.230	ml/mol	McGowan Method
pc	975.34	kPa	Joback Method
rinpol	2883.00		NIST Webbook
tb	955.20	K	Joback Method
tc	1169.50	K	Joback Method
tf	539.77	K	Joback Method
vc	1.369	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1181.72	J/molxK	955.20	Joback Method
cpg	1198.96	J/molxK	990.92	Joback Method
cpg	1214.75	J/molxK	1026.63	Joback Method
cpg	1229.11	J/molxK	1062.35	Joback Method
cpg	1242.11	J/molxK	1098.07	Joback Method
cpg	1253.77	J/molxK	1133.79	Joback Method
cpg	1264.15	J/molxK	1169.50	Joback Method
dvisc	0.0003804	Paxs	539.77	Joback Method
dvisc	0.0001851	Paxs	609.01	Joback Method

dvisc	0.0001043	Paxs	678.25	Joback Method
dvisc	0.0000654	Paxs	747.48	Joback Method
dvisc	0.0000443	Paxs	816.72	Joback Method
dvisc	0.0000320	Paxs	885.96	Joback Method
dvisc	0.0000242	Paxs	955.20	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=U355053&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355053&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>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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