

# Succinic acid, tridec-2-yn-1-yl 2-naphthyl ester

**Inchi:** InChI=1S/C27H34O4/c1-2-3-4-5-6-7-8-9-10-11-14-21-30-26(28)19-20-27(29)31-25-18-17  
**InchiKey:** DXNUIJNUJXTUDK-UHFFFAOYSA-N  
**Formula:** C27H34O4  
**SMILES:** CCCCCCCCCC#CCOC(=O)CCC(=O)Oc1ccc2ccccc2c1  
**Mol. weight [g/mol]:** 422.56

## Physical Properties

Property code	Value	Unit	Source
gf	120.85	kJ/mol	Joback Method
hf	-401.78	kJ/mol	Joback Method
hfus	65.05	kJ/mol	Joback Method
hvap	100.74	kJ/mol	Joback Method
log10ws	-8.53		Crippen Method
logp	6.603		Crippen Method
mvol	354.350	ml/mol	McGowan Method
pc	1113.34	kPa	Joback Method
rinpol	3473.00		NIST Webbook
rinpol	3473.00		NIST Webbook
tb	1029.38	K	Joback Method
tc	1261.43	K	Joback Method
tf	716.11	K	Joback Method
vc	1.371	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1166.24	J/mol×K	1029.38	Joback Method
cpg	1181.39	J/mol×K	1068.06	Joback Method
cpg	1195.29	J/mol×K	1106.73	Joback Method
cpg	1208.04	J/mol×K	1145.41	Joback Method
cpg	1219.71	J/mol×K	1184.08	Joback Method
cpg	1230.39	J/mol×K	1222.76	Joback Method
cpg	1240.17	J/mol×K	1261.43	Joback Method

# Sources

<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=U389844&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U389844&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>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>rinpolar:</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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