

# Succinic acid, 4-methylthiophenyl nonyl ester

**Inchi:** InChI=1S/C20H30O4S/c1-3-4-5-6-7-8-9-16-23-19(21)14-15-20(22)24-17-10-12-18(25-2)  
**InchiKey:** HNEFUMZYQUILQI-UHFFFAOYSA-N  
**Formula:** C20H30O4S  
**SMILES:** CCCCCCCCCOC(=O)CCC(=O)Oc1ccc(SC)cc1  
**Mol. weight [g/mol]:** 366.51

## Physical Properties

Property code	Value	Unit	Source
gf	-214.42	kJ/mol	Joback Method
hf	-678.80	kJ/mol	Joback Method
hfus	50.91	kJ/mol	Joback Method
hvap	88.18	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.388		Crippen Method
mcvol	300.130	ml/mol	McGowan Method
pc	1358.63	kPa	Joback Method
rinpol	2809.00		NIST Webbook
rinpol	2809.00		NIST Webbook
tb	910.02	K	Joback Method
tc	1123.46	K	Joback Method
tf	532.82	K	Joback Method
vc	1.149	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	936.75	J/mol×K	910.02	Joback Method
cpg	951.39	J/mol×K	945.59	Joback Method
cpg	964.69	J/mol×K	981.17	Joback Method
cpg	976.70	J/mol×K	1016.74	Joback Method
cpg	987.41	J/mol×K	1052.31	Joback Method
cpg	996.85	J/mol×K	1087.89	Joback Method
cpg	1005.05	J/mol×K	1123.46	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U380913&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380913&amp;Units=SI</a>
<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>

# 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>hvp:</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>rinp:</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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