

# Succinic acid, dodecyl 4-methylthiophenyl ester

<b>Inchi:</b>	InChI=1S/C23H36O4S/c1-3-4-5-6-7-8-9-10-11-12-19-26-22(24)17-18-23(25)27-20-13-15
<b>InchiKey:</b>	UWAPJZRMYYQRHA-UHFFFAOYSA-N
<b>Formula:</b>	C23H36O4S
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)CCC(=O)Oc1ccc(SC)cc1
<b>Mol. weight [g/mol]:</b>	408.60

## Physical Properties

Property code	Value	Unit	Source
gf	-189.16	kJ/mol	Joback Method
hf	-740.72	kJ/mol	Joback Method
hfus	58.68	kJ/mol	Joback Method
hvap	94.86	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	6.558		Crippen Method
mvol	342.400	ml/mol	McGowan Method
pc	1110.37	kPa	Joback Method
rinpol	3103.00		NIST Webbook
rinpol	3103.00		NIST Webbook
tb	978.66	K	Joback Method
tc	1199.12	K	Joback Method
tf	566.63	K	Joback Method
vc	1.317	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1117.15	J/molxK	978.66	Joback Method
cpg	1132.04	J/molxK	1015.40	Joback Method
cpg	1145.41	J/molxK	1052.15	Joback Method
cpg	1157.30	J/molxK	1088.89	Joback Method
cpg	1167.73	J/molxK	1125.64	Joback Method
cpg	1176.73	J/molxK	1162.38	Joback Method
cpg	1184.33	J/molxK	1199.12	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=U380916&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380916&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>h vap:</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>r in pol:</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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