

# Succinic acid, butyl 4-methylthiophenyl ester

<b>Inchi:</b>	InChI=1S/C15H20O4S/c1-3-4-11-18-14(16)9-10-15(17)19-12-5-7-13(20-2)8-6-12/h5-8H,
<b>InchiKey:</b>	BYGUVFIJQCCIMQ-UHFFFAOYSA-N
<b>Formula:</b>	C15H20O4S
<b>SMILES:</b>	CCCCOC(=O)CCC(=O)Oc1ccc(SC)cc1
<b>Mol. weight [g/mol]:</b>	296.38

## Physical Properties

Property code	Value	Unit	Source
gf	-256.52	kJ/mol	Joback Method
hf	-575.60	kJ/mol	Joback Method
hfus	37.96	kJ/mol	Joback Method
hvap	77.05	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.437		Crippen Method
mvol	229.680	ml/mol	McGowan Method
pc	2005.50	kPa	Joback Method
rinpol	2300.00		NIST Webbook
rinpol	2300.00		NIST Webbook
tb	795.62	K	Joback Method
tc	1012.87	K	Joback Method
tf	476.47	K	Joback Method
vc	0.870	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.30	J/mol×K	795.62	Joback Method
cpg	663.21	J/mol×K	831.83	Joback Method
cpg	676.01	J/mol×K	868.04	Joback Method
cpg	687.69	J/mol×K	904.24	Joback Method
cpg	698.26	J/mol×K	940.45	Joback Method
cpg	707.73	J/mol×K	976.66	Joback Method
cpg	716.10	J/mol×K	1012.87	Joback Method

# Sources

<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=U380907&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380907&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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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