

# Succinic acid, isobutyl 4-methylthiophenyl ester

Inchi:	InChI=1S/C15H20O4S/c1-11(2)10-18-14(16)8-9-15(17)19-12-4-6-13(20-3)7-5-12/h4-7,1
InchiKey:	CKQKBWJIDRXIHN-UHFFFAOYSA-N
Formula:	C15H20O4S
SMILES:	CSc1ccc(OC(=O)CCC(=O)OCC(C)C)cc1
Mol. weight [g/mol]:	296.38

## Physical Properties

Property code	Value	Unit	Source
gf	-258.96	kJ/mol	Joback Method
hf	-580.88	kJ/mol	Joback Method
hfus	34.44	kJ/mol	Joback Method
hvap	76.66	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.293		Crippen Method
mvol	229.680	ml/mol	McGowan Method
pc	2019.95	kPa	Joback Method
rinpol	2257.00		NIST Webbook
rinpol	2257.00		NIST Webbook
tb	795.18	K	Joback Method
tc	1015.72	K	Joback Method
tf	461.47	K	Joback Method
vc	0.864	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.88	J/mol×K	795.18	Joback Method
cpg	663.99	J/mol×K	831.94	Joback Method
cpg	676.95	J/mol×K	868.69	Joback Method
cpg	688.74	J/mol×K	905.45	Joback Method
cpg	699.38	J/mol×K	942.20	Joback Method
cpg	708.88	J/mol×K	978.96	Joback Method
cpg	717.22	J/mol×K	1015.72	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U380906&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380906&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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