

# Terephthalic acid, isobutyl 4-methylthiophenyl ester

<b>Inchi:</b>	InChI=1S/C19H20O4S/c1-13(2)12-22-18(20)14-4-6-15(7-5-14)19(21)23-16-8-10-17(24-3
<b>InchiKey:</b>	JTFYCFZJDIWATP-UHFFFAOYSA-N
<b>Formula:</b>	C19H20O4S
<b>SMILES:</b>	CSc1ccc(OC(=O)c2ccc(C(=O)OCC(C)C)cc2)cc1
<b>Mol. weight [g/mol]:</b>	344.43

## Physical Properties

Property code	Value	Unit	Source
gf	-122.50	kJ/mol	Joback Method
hf	-438.38	kJ/mol	Joback Method
hfus	38.45	kJ/mol	Joback Method
hvap	88.50	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	4.440		Crippen Method
mcvol	262.280	ml/mol	McGowan Method
pc	1901.92	kPa	Joback Method
rinpola	2912.00		NIST Webbook
rinpola	2912.00		NIST Webbook
tb	918.36	K	Joback Method
tc	1160.99	K	Joback Method
tf	545.49	K	Joback Method
vc	0.980	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	775.28	J/molxK	918.36	Joback Method
cpg	787.61	J/molxK	958.80	Joback Method
cpg	798.40	J/molxK	999.24	Joback Method
cpg	807.69	J/molxK	1039.68	Joback Method
cpg	815.49	J/molxK	1080.11	Joback Method
cpg	821.83	J/molxK	1120.55	Joback Method
cpg	826.74	J/molxK	1160.99	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U416120&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416120&amp;Units=SI</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>rinpola:</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

Latest version available from:

<https://www.chemeo.com/cid/97-830-3/Terephthalic-acid-isobutyl-4-methylthiophenyl-ester.pdf>

Generated by Cheméo on 2024-04-28 23:25:48.622995989 +0000 UTC m=+16635997.543573300.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.