

# Terephthalic acid, isohexyl 4-methylthiophenyl ester

<b>Inchi:</b>	InChI=1S/C21H24O4S/c1-15(2)5-4-14-24-20(22)16-6-8-17(9-7-16)21(23)25-18-10-12-19
<b>InchiKey:</b>	XUAZSXDZFCCTR-UHFFFAOYSA-N
<b>Formula:</b>	C21H24O4S
<b>SMILES:</b>	CSc1ccc(OC(=O)c2ccc(C(=O)OCCCC(C)C)cc2)cc1
<b>Mol. weight [g/mol]:</b>	372.48

## Physical Properties

Property code	Value	Unit	Source
gf	-105.66	kJ/mol	Joback Method
hf	-479.66	kJ/mol	Joback Method
hfus	43.63	kJ/mol	Joback Method
hvap	92.96	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	5.221		Crippen Method
mvol	290.460	ml/mol	McGowan Method
pc	1619.37	kPa	Joback Method
rinpol	3130.00		NIST Webbook
rinpol	3130.00		NIST Webbook
tb	964.12	K	Joback Method
tc	1202.55	K	Joback Method
tf	568.03	K	Joback Method
vc	1.091	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	890.68	J/mol×K	964.12	Joback Method
cpg	902.89	J/mol×K	1003.86	Joback Method
cpg	913.53	J/mol×K	1043.60	Joback Method
cpg	922.64	J/mol×K	1083.34	Joback Method
cpg	930.23	J/mol×K	1123.08	Joback Method
cpg	936.35	J/mol×K	1162.82	Joback Method
cpg	941.03	J/mol×K	1202.55	Joback Method

# Sources

<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=U416123&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416123&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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

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