

# Diethylmalonic acid, 2-methylthiophenyl nonyl ester

<b>Inchi:</b>	InChI=1S/C23H36O4S/c1-5-8-9-10-11-12-15-18-26-21(24)23(6-2,7-3)22(25)27-19-16-13
<b>InchiKey:</b>	ZOMSKPCGXGZNIL-UHFFFAOYSA-N
<b>Formula:</b>	C23H36O4S
<b>SMILES:</b>	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1SC
<b>Mol. weight [g/mol]:</b>	408.60

## Physical Properties

Property code	Value	Unit	Source
gf	-186.32	kJ/mol	Joback Method
hf	-749.47	kJ/mol	Joback Method
hfus	51.27	kJ/mol	Joback Method
hvap	93.56	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	6.414		Crippen Method
mvol	342.400	ml/mol	McGowan Method
pc	1124.57	kPa	Joback Method
rinpol	2759.00		NIST Webbook
rinpol	2759.00		NIST Webbook
tb	975.43	K	Joback Method
tc	1197.51	K	Joback Method
tf	569.05	K	Joback Method
vc	1.306	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1117.30	J/molxK	975.43	Joback Method
cpg	1132.35	J/molxK	1012.44	Joback Method
cpg	1145.97	J/molxK	1049.46	Joback Method
cpg	1158.22	J/molxK	1086.47	Joback Method
cpg	1169.17	J/molxK	1123.48	Joback Method
cpg	1178.86	J/molxK	1160.49	Joback Method
cpg	1187.36	J/molxK	1197.51	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.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>
<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=U369536&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369536&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>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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