

# Methyl tridecyl phthalate

<b>Other names:</b>	1,2-Benzenedicarboxylic acid, tridecyl methyl ester
<b>Inchi:</b>	InChI=1S/C22H34O4/c1-3-4-5-6-7-8-9-10-11-12-15-18-26-22(24)20-17-14-13-16-19(20)
<b>InchiKey:</b>	AWBAYRSFSGKGS-UHFFFAOYSA-N
<b>Formula:</b>	C22H34O4
<b>SMILES:</b>	CCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OC
<b>Mol. weight [g/mol]:</b>	362.50
<b>CAS:</b>	256481-40-0

## Physical Properties

Property code	Value	Unit	Source
gf	-230.70	kJ/mol	Joback Method
hf	-761.95	kJ/mol	Joback Method
hfus	51.96	kJ/mol	Joback Method
hvap	85.82	kJ/mol	Joback Method
log10ws	-6.98		Crippen Method
logp	5.941		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1171.22	kPa	Joback Method
rinpol	2654.00		NIST Webbook
tb	887.00	K	Joback Method
tc	1090.20	K	Joback Method
tf	520.96	K	Joback Method
vc	1.208	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.29	J/mol×K	887.00	Joback Method
cpg	1013.85	J/mol×K	920.87	Joback Method
cpg	1029.18	J/mol×K	954.73	Joback Method
cpg	1043.31	J/mol×K	988.60	Joback Method
cpg	1056.27	J/mol×K	1022.47	Joback Method
cpg	1068.08	J/mol×K	1056.33	Joback Method
cpg	1078.77	J/mol×K	1090.20	Joback Method

dvisc	0.0004813	Paxs	520.96	Joback Method
dvisc	0.0002579	Paxs	581.97	Joback Method
dvisc	0.0001556	Paxs	642.97	Joback Method
dvisc	0.0001024	Paxs	703.98	Joback Method
dvisc	0.0000721	Paxs	764.99	Joback Method
dvisc	0.0000534	Paxs	825.99	Joback Method
dvisc	0.0000413	Paxs	887.00	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C256481400&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C256481400&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>dvisc:</b>	Dynamic viscosity
<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>mvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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