

# o-Toluic acid, 3-tridecyl ester

<b>Other names:</b>	o-Toluylic acid, 3-tridecyl ester
<b>Inchi:</b>	InChI=1S/C21H34O2/c1-4-6-7-8-9-10-11-12-16-19(5-2)23-21(22)20-17-14-13-15-18(20)3
<b>InchiKey:</b>	GBBVVIGLDIOKSI-UHFFFAOYSA-N
<b>Formula:</b>	C21H34O2
<b>SMILES:</b>	CCCCCCCCCCC(CC)OC(=O)c1ccccc1C
<b>Mol. weight [g/mol]:</b>	318.49

## Physical Properties

Property code	Value	Unit	Source
gf	-7.64	kJ/mol	Joback Method
hf	-501.79	kJ/mol	Joback Method
hfus	43.06	kJ/mol	Joback Method
hvap	74.05	kJ/mol	Joback Method
log10ws	-7.32		Crippen Method
logp	6.461		Crippen Method
mvol	290.430	ml/mol	McGowan Method
pc	1219.14	kPa	Joback Method
rinpol	2206.00		NIST Webbook
rinpol	2206.00		NIST Webbook
tb	787.39	K	Joback Method
tc	980.88	K	Joback Method
tf	422.53	K	Joback Method
vc	1.121	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.66	J/mol×K	787.39	Joback Method
cpg	968.16	J/mol×K	948.63	Joback Method
cpg	953.71	J/mol×K	916.38	Joback Method
cpg	938.27	J/mol×K	884.13	Joback Method
cpg	921.80	J/mol×K	851.89	Joback Method
cpg	904.28	J/mol×K	819.64	Joback Method
cpg	981.66	J/mol×K	980.88	Joback Method

dvisc	0.0000601	Paxs	787.39	Joback Method
dvisc	0.0000799	Paxs	726.58	Joback Method
dvisc	0.0001118	Paxs	665.77	Joback Method
dvisc	0.0001674	Paxs	604.96	Joback Method
dvisc	0.0002745	Paxs	544.15	Joback Method
dvisc	0.0005097	Paxs	483.34	Joback Method
dvisc	0.0011307	Paxs	422.53	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=U299791&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299791&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>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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