

# Oxanilic acid, 2-tert-butyl-, ethyl ester

<b>Inchi:</b>	InChI=1S/C14H19NO3/c1-5-18-13(17)12(16)15-11-9-7-6-8-10(11)14(2,3)4/h6-9H,5H2,1-
<b>InchiKey:</b>	DPFZZLSEANVIOP-UHFFFAOYSA-N
<b>Formula:</b>	C14H19NO3
<b>SMILES:</b>	CCOC(=O)C(=O)Nc1cccc1C(C)(C)C
<b>Mol. weight [g/mol]:</b>	249.31

## Physical Properties

Property code	Value	Unit	Source
gf	-100.83	kJ/mol	Joback Method
hf	-419.89	kJ/mol	Joback Method
hfus	27.74	kJ/mol	Joback Method
hvap	70.74	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.486		Crippen Method
mvol	203.350	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
tb	728.48	K	Joback Method
tc	946.32	K	Joback Method
tf	463.65	K	Joback Method
vc	0.765	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.55	J/molxK	728.48	Joback Method
cpg	584.06	J/molxK	764.79	Joback Method
cpg	597.52	J/molxK	801.09	Joback Method
cpg	609.99	J/molxK	837.40	Joback Method
cpg	621.51	J/molxK	873.71	Joback Method
cpg	632.14	J/molxK	910.01	Joback Method
cpg	641.92	J/molxK	946.32	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009255&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009255&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>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>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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