

# 3«beta»-Tigloyloxynortropane

<b>Inchi:</b>	InChI=1S/C12H19NO2/c1-3-8(2)12(14)15-11-6-9-4-5-10(7-11)13-9/h3,9-11,13H,4-7H2,1
<b>InchiKey:</b>	KLFGVBUPYUSQKV-FPYGCLRLSA-N
<b>Formula:</b>	C12H19NO2
<b>SMILES:</b>	CC=C(C)C(=O)OC1CC2CCC(C1)N2
<b>Mol. weight [g/mol]:</b>	209.28
<b>CAS:</b>	855980-78-8

## Physical Properties

Property code	Value	Unit	Source
gf	65.21	kJ/mol	Joback Method
hf	-277.63	kJ/mol	Joback Method
hfus	31.25	kJ/mol	Joback Method
hvap	58.12	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	1.779		Crippen Method
mcvol	171.340	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
rinpol	1936.30		NIST Webbook
tb	620.19	K	Joback Method
tc	843.33	K	Joback Method
tf	407.75	K	Joback Method
vc	0.646	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.99	J/molxK	620.19	Joback Method
cpg	489.95	J/molxK	657.38	Joback Method
cpg	507.71	J/molxK	694.57	Joback Method
cpg	524.33	J/molxK	731.76	Joback Method
cpg	539.88	J/molxK	768.95	Joback Method
cpg	554.41	J/molxK	806.14	Joback Method
cpg	567.98	J/molxK	843.33	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C855980788&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C855980788&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>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

Latest version available from:

<https://www.chemeo.com/cid/75-581-4/3-beta-Tigloyloxynortropane.pdf>

Generated by Cheméo on 2024-04-19 17:07:10.302639443 +0000 UTC m=+15835679.223216756.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.