

# T-2 toxin

<b>Inchi:</b>	InChI=1S/C24H34O9/c1-12(2)7-18(27)32-16-9-23(10-29-14(4)25)17(8-13(16)3)33-21-19
<b>InchiKey:</b>	BXFOFFBJRFZBQZ-GUBDHGAJSA-N
<b>Formula:</b>	C24H34O9
<b>SMILES:</b>	CC(=O)OCC12CC(OC(=O)CC(C)C)C(C)=CC1OC1C(O)C(OC(C)=O)C2(C)C12CO2
<b>Mol. weight [g/mol]:</b>	466.52

## Physical Properties

Property code	Value	Unit	Source
gf	-670.24	kJ/mol	Joback Method
hf	-1405.05	kJ/mol	Joback Method
hfus	57.36	kJ/mol	Joback Method
hvap	118.06	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	1.693		Crippen Method
mcvol	341.210	ml/mol	McGowan Method
pc	1363.65	kPa	Joback Method
rinpol	2822.00		NIST Webbook
rinpol	2822.00		NIST Webbook
rinpol	2822.00		NIST Webbook
tb	1144.71	K	Joback Method
tc	1403.04	K	Joback Method
tf	808.42	K	Joback Method
vc	1.294	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1410.70	J/molxK	1144.71	Joback Method
cpg	1458.52	J/molxK	1187.77	Joback Method
cpg	1510.77	J/molxK	1230.82	Joback Method
cpg	1568.02	J/molxK	1273.88	Joback Method
cpg	1630.83	J/molxK	1316.93	Joback Method
cpg	1699.75	J/molxK	1359.99	Joback Method
cpg	1775.35	J/molxK	1403.04	Joback Method

# Sources

<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=R75151&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R75151&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>h vap:</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>r in pol:</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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