

# 4H-1,2-Diazepine, 3,5,7-triphenyl-

<b>Other names:</b>	3,5,7-Triphenyl-4H-1,2-diazepine 3,5,7-Triphenyl-1,2-diazepin 3,5,7-Triphenyl-1,2-diazepine
<b>Inchi:</b>	InChI=1S/C23H18N2/c1-4-10-18(11-5-1)21-16-22(19-12-6-2-7-13-19)24-25-23(17-21)20
<b>InchiKey:</b>	NCJIYZKOKVSKDJ-UHFFFAOYSA-N
<b>Formula:</b>	C23H18N2
<b>SMILES:</b>	<chem>C1=C(c2ccccc2)CC(c2ccccc2)=NN=C1c1ccccc1</chem>
<b>Mol. weight [g/mol]:</b>	322.40
<b>CAS:</b>	25649-70-1

## Physical Properties

Property code	Value	Unit	Source
gf	794.62	kJ/mol	Joback Method
hf	540.91	kJ/mol	Joback Method
hfus	38.89	kJ/mol	Joback Method
hvap	89.81	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.367		Crippen Method
mcvol	259.850	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
tb	953.99	K	Joback Method
tc	1255.38	K	Joback Method
tf	619.25	K	Joback Method
vc	0.982	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.81	J/molxK	953.99	Joback Method
cpg	837.88	J/molxK	1004.22	Joback Method
cpg	849.27	J/molxK	1054.45	Joback Method
cpg	858.10	J/molxK	1104.68	Joback Method
cpg	864.51	J/molxK	1154.91	Joback Method
cpg	868.60	J/molxK	1205.14	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C25649701&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C25649701&amp;Units=SI</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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