

# Benzene, 1,1'-(2-nitropropylidene)bis[4-chloro-

<b>Other names:</b>	Propane, 1,1-bis(p-chlorophenyl)-2-nitro- CS 645A DNP Prolan 1,1-Bis(p-Chlorophenyl)-2-nitropropane 2-Nitro-1,1-bis(p-chlorophenyl)propane 1,1-Bis(4-chlorophenyl)-2-nitropropane ENT 22,784 1,1'-(2-Nitropropylidene)bis(4-chlorobenzene) Prolan (insecticide) 1,1-(Di-p-chlorophenyl)-2-nitropropane
<b>Inchi:</b>	InChI=1S/C15H13Cl2NO2/c1-10(18(19)20)15(11-2-6-13(16)7-3-11)12-4-8-14(17)9-5-12/
<b>InchiKey:</b>	JCWVUDIGEJLVPS-UHFFFAOYSA-N
<b>Formula:</b>	C15H13Cl2NO2
<b>SMILES:</b>	CC(C(c1ccc(Cl)cc1)c1ccc(Cl)cc1)[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	310.18
<b>CAS:</b>	117-27-1

## Physical Properties

Property code	Value	Unit	Source
gf	287.79	kJ/mol	Joback Method
hf	44.39	kJ/mol	Joback Method
hfus	34.62	kJ/mol	Joback Method
hvap	79.45	kJ/mol	Joback Method
log10ws	-5.94		Crippen Method
logp	4.790		Crippen Method
mcvol	216.590	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
rinpol	2250.00		NIST Webbook
rinpol	2250.00		NIST Webbook
rinpol	2250.00		NIST Webbook
tb	831.74	K	Joback Method
tc	1101.27	K	Joback Method
tf	355.17 ± 0.20	K	NIST Webbook
vc	0.828	m3/kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.69	J/mol×K	831.74	Joback Method
cpg	585.30	J/mol×K	876.66	Joback Method
cpg	596.68	J/mol×K	921.58	Joback Method
cpg	606.93	J/mol×K	966.51	Joback Method
cpg	616.17	J/mol×K	1011.43	Joback Method
cpg	624.51	J/mol×K	1056.35	Joback Method
cpg	632.06	J/mol×K	1101.27	Joback Method
hfust	21.39	kJ/mol	354.30	NIST Webbook

## 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=C117271&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C117271&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>

## 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>hfust:</b>	Enthalpy of fusion at a given temperature
<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>mccvol:</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

**vc:** Critical Volume

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