

# 1,1':4',1''-Terphenyl, 4-nitro-

<b>Other names:</b>	4-Nitro-p-terphenyl p-Terphenyl, 4-nitro- 4-Nitro-(para-terphenyl) 4-nitro-1,1':4':1''-terphenyl
<b>Inchi:</b>	InChI=1S/C18H13NO2/c20-19(21)18-12-10-17(11-13-18)16-8-6-15(7-9-16)14-4-2-1-3-5-
<b>InchiKey:</b>	IMMGNSJGTWWGJB-UHFFFAOYSA-N
<b>Formula:</b>	C18H13NO2
<b>SMILES:</b>	O=[N+]([O-])c1ccc(-c2ccc(-c3ccccc3)cc2)cc1
<b>Mol. weight [g/mol]:</b>	275.30
<b>CAS:</b>	10355-53-0

## Physical Properties

Property code	Value	Unit	Source
gf	454.20	kJ/mol	Joback Method
hf	261.04	kJ/mol	Joback Method
hfus	35.08	kJ/mol	Joback Method
hvap	80.41	kJ/mol	Joback Method
log10ws	-7.33		Crippen Method
logp	4.929		Crippen Method
mcvol	210.620	ml/mol	McGowan Method
pc	2574.11	kPa	Joback Method
rinpol	2695.00		NIST Webbook
rinpol	2696.00		NIST Webbook
rinpol	437.81		NIST Webbook
rinpol	443.20		NIST Webbook
rinpol	2654.00		NIST Webbook
rinpol	2696.00		NIST Webbook
rinpol	2696.00		NIST Webbook
rinpol	443.20		NIST Webbook
tb	853.08	K	Joback Method
tc	1139.20	K	Joback Method
tf	540.53	K	Joback Method
vc	0.801	m3/kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.24	J/mol×K	853.08	Joback Method
cpg	608.12	J/mol×K	900.77	Joback Method
cpg	620.55	J/mol×K	948.45	Joback Method
cpg	631.69	J/mol×K	996.14	Joback Method
cpg	641.70	J/mol×K	1043.83	Joback Method
cpg	650.75	J/mol×K	1091.51	Joback Method
cpg	659.00	J/mol×K	1139.20	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=C10355530&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C10355530&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>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
<b>vc:</b>	Critical Volume

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