

# Benzene, 2,4-dinitro-1-(2-phenylethenyl)-

<b>Other names:</b>	Stilbene, 2,4-dinitro- 2,4-Dinitrostilbene
<b>Inchi:</b>	InChI=1S/C14H10N2O4/c17-15(18)13-9-8-12(14(10-13)16(19)20)7-6-11-4-2-1-3-5-11/h1
<b>InchiKey:</b>	YHUVJTKXOKHAQP-VOTSOKGWSA-N
<b>Formula:</b>	C14H10N2O4
<b>SMILES:</b>	O=[N+]([O-])c1ccc(C=Cc2ccccc2)c([N+] (=O)[O-])c1
<b>Mol. weight [g/mol]:</b>	270.24
<b>CAS:</b>	2486-13-7

## Physical Properties

Property code	Value	Unit	Source
gf	423.88	kJ/mol	Joback Method
hf	213.53	kJ/mol	Joback Method
hfus	42.24	kJ/mol	Joback Method
hvap	85.77	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	3.673		Crippen Method
mcvol	191.140	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
tb	890.88	K	Joback Method
tc	1178.34	K	Joback Method
tf	607.56	K	Joback Method
vc	0.748	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.87	J/molxK	890.88	Joback Method
cpg	547.82	J/molxK	938.79	Joback Method
cpg	557.75	J/molxK	986.70	Joback Method
cpg	566.83	J/molxK	1034.61	Joback Method
cpg	575.22	J/molxK	1082.52	Joback Method
cpg	583.08	J/molxK	1130.43	Joback Method
cpg	590.57	J/molxK	1178.34	Joback Method

# 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=C2486137&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2486137&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>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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