

TRANS-4-NITROSTILBENE

Other names:	trans-p-Nitrostilbene trans-4-Nitrostilbene Benzene, 1-nitro-4-(2-phenylethenyl)-, (E)- Stilbene, 4-nitro-, (E)- 4-Nitrostilbene, trans 4-Nitro-trans-stilbene trans-4-Mononitrostilbene
Inchi:	InChI=1S/C14H11NO2/c16-15(17)14-10-8-13(9-11-14)7-6-12-4-2-1-3-5-12/h1-11H/b7-6-
InchiKey:	ZISCOWXWCHUSMH-VOTSOKGWSA-N
Formula:	C14H11NO2
SMILES:	O=[N+][O-]c1ccc(/C=C/c2ccccc2)cc1
Mol. weight [g/mol]:	225.25

Physical Properties

Property code	Value	Unit	Source
chs	-7183.90 ± 2.90	kJ/mol	NIST Webbook
hf	206.79	kJ/mol	Cheméo Relay (1.0)
hfs	102.70 ± 3.00	kJ/mol	NIST Webbook
hfus	31.27	kJ/mol	Joback Method
hvap	99.76	kJ/mol	Cheméo Relay (1.0)
ie	8.32	eV	Cheméo Relay (1.0)
log10ws	-4.96		Cheméo Relay (1.0)
logp	3.765		Crippen Method
mcvol	173.720	ml/mol	McGowan Method
tb	633.48	K	Cheméo Relay (1.0)
tf	445.55	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.07	J/mol×K	734.06	Joback Method
cpg	465.08	J/mol×K	779.54	Joback Method
cpg	477.79	J/mol×K	825.01	Joback Method
cpg	489.35	J/mol×K	870.49	Joback Method

cpg	499.89	J/mol×K	915.97	Joback Method
cpg	509.55	J/mol×K	961.45	Joback Method
cpg	518.48	J/mol×K	1006.92	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1694208&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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