Benzene, 1,1'-(1,2-ethenediyl)bis[2,4,6-trinitro-

Other names:	1,1'-(1,2-Ethenediyl)bis(2,4,6-trinitrobenzene)
	2,2',4,4',6,6'-hexanitrostilbene
	HNS
	HNS(2,2',4,4',6,6'-hexanitrostilbene)
	Stilbene, 2,2',4,4',6,6'-hexanitro-
Inchi:	InChI=1S/C14H6N6O12/c21-15(22)7-3-11(17(25)26)9(12(4-7)18(27)28)1-2-10-13(19(29)
InchiKey:	YSIBQULRFXITSW-OWOJBTEDSA-N
Formula:	C14H6N6O12
SMILES:	O=[N+]([O-])c1cc([N+](=O)[O-])c(C=Cc2c([N+](=O)[O-])cc([N+](=O)[O-])cc2[N+](=O)[O-])c
Mol. weight [g/mol]:	450.23
CAS:	20062-22-0

Physical Properties

Property code	Value	Unit	Source
chs	-6434.20 ± 5.00	kJ/mol	NIST Webbook
chs	-6424.70 ± 4.50	kJ/mol	NIST Webbook
gf	527.56	kJ/mol	Joback Method
hf	238.40	kJ/mol	NIST Webbook
hfs	58.07	kJ/mol	NIST Webbook
hfs	68.00 ± 10.00	kJ/mol	NIST Webbook
hfus	86.13	kJ/mol	Joback Method
hvap	154.79	kJ/mol	Joback Method
log10ws	-7.98		Crippen Method
logp	3.306		Crippen Method
mcvol	260.820	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
tb	1518.16	K	Joback Method
tc	1863.76	K	Joback Method
tf	1232.08	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	792.16	J/mol×K	1518.16	Joback Method
cpg	797.45	J/mol×K	1575.76	Joback Method
cpg	803.42	J/mol×K	1633.36	Joback Method
cpg	810.33	J/mol×K	1690.96	Joback Method
cpg	818.44	J/mol×K	1748.56	Joback Method
cpg	828.00	J/mol×K	1806.16	Joback Method
cpg	839.27	J/mol×K	1863.76	Joback Method
hsubt	179.90	kJ/mol	456.50	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20062220&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of 2,2',4,4',6,6'-hexanitrostilbene in binary solvent of N,N-dimethylformamide and acetonitrile:	https://www.doi.org/10.1016/j.jct.2015.12.004

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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