

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

Other names:	Stilbene, 2,4-dinitro- 2,4-Dinitrostilbene
Inchi:	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
InchiKey:	YHUVJTKXOKHAQP-VOTSOKGWSA-N
Formula:	C14H10N2O4
SMILES:	O=[N+]([O-])c1ccc(C=Cc2ccccc2)c([N+] (=O) [O-])c1
Mol. weight [g/mol]:	270.24
CAS:	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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2486137&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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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