1,1'-ETHYLENEBIS(2-NITROBENZENE)

Other names: Benzene, 1,1'-(1,2-ethanediyl)bis[2-nitro-
Bibenzyl, 2,2'-dinitro-
Dinitro-2,2' dibenzyl
o,o'-dinitrobibenzyl
Inchi: InChI=1S/C14H12N2O4/c17-15(18)13-7-3-1-5-11(13)9-10-12-6-2-4-8-14(12)16(19)20/h1
InchiKey: YBOZRPPSBVIHGJ-UHFFFAOYSA-N
Formula: C14H12N2O4
SMILES: O=[N+]([O-])c1ccccc1CCc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 272.26

Physical Properties

Property code	Value	Unit	Source
hf	136.36	kJ/mol	Cheméo Relay (1.0)
hfus	42.04	kJ/mol	Joback Method
hvap	106.51	kJ/mol	Cheméo Relay (1.0)
ie	9.43	eV	Cheméo Relay (1.0)
log10ws	-4.87		Cheméo Relay (1.0)
logp	3.288		Crippen Method
mcvol	195.440	ml/mol	McGowan Method
rinpol	372.85		NIST Webbook
rinpol	372.85		NIST Webbook
tb	618.71	K	Cheméo Relay (1.0)
tf	359.41	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.16	J/mol×K	886.72	Joback Method
cpg	576.51	J/mol×K	932.93	Joback Method
cpg	586.69	J/mol×K	979.13	Joback Method
cpg	595.81	J/mol×K	1025.34	Joback Method
cpg	604.00	J/mol×K	1071.54	Joback Method
cpg	611.37	J/mol×K	1117.75	Joback Method
cpg	618.04	J/mol×K	1163.96	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16968197&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

cpg:	Ideal gas heat capacity
hf:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point