1,1'-METHYLENEBIS(4-NITROBENZENE)

Other names:	Methane, bis(p-nitrophenyl)-
	Bis(p-nitrophenyl)methane
	Bis(4-nitrophenyl)methane
	4,4'-Dinitrodiphenylmethane
	Benzene, 1,1'-methylenebis*4-nitro-
Inchi:	InChI=1S/C13H10N2O4/c16-14(17)12-5-1-10(2-6-12)9-11-3-7-13(8-4-11)15(18)19/h1-8H
InchiKey:	GLBZQZXDUTUCGK-UHFFFAOYSA-N
Formula:	C13H10N2O4
SMILES:	O=[N+]([O-])c1ccc(Cc2ccc([N+](=O)[O-])cc2)cc1
Mol. weight [g/mol]:	258.23

Physical Properties

Property code	Value	Unit	Source
hf	151.57	kJ/mol	Cheméo Relay (1.0)
hfus	39.45	kJ/mol	Joback Method
hvap	108.79	kJ/mol	Cheméo Relay (1.0)
ie	9.98 ± 0.05	eV	NIST Webbook
log10ws	-4.70		Cheméo Relay (1.0)
logp	3.094		Crippen Method
mcvol	181.350	ml/mol	McGowan Method
tb	633.29	K	Cheméo Relay (1.0)
tf	384.04	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.84	J/mol×K	863.84	Joback Method
cpg	521.82	J/mol×K	911.17	Joback Method
cpg	531.63	J/mol×K	958.50	Joback Method
cpg	540.36	J/mol×K	1005.83	Joback Method
cpg	548.15	J/mol×K	1053.16	Joback Method
cpg	555.09	J/mol×K	1100.49	Joback Method
cpg	561.33	J/mol×K	1147.82	Joback Method

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1817749&Units=SI

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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point