

Benzene, 1,1'-methylenebis[4-nitro-

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
CAS:	1817-74-9

Physical Properties

Property code	Value	Unit	Source
gf	335.24	kJ/mol	Joback Method
hf	116.95	kJ/mol	Joback Method
hfus	39.45	kJ/mol	Joback Method
hvap	83.59	kJ/mol	Joback Method
ie	9.98 ± 0.05	eV	NIST Webbook
log10ws	-4.87		Crippen Method
logp	3.094		Crippen Method
mcvol	181.350	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
tb	863.84	K	Joback Method
tc	1147.82	K	Joback Method
tf	601.37	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.84	J/molxK	863.84	Joback Method
cpg	521.82	J/molxK	911.17	Joback Method
cpg	531.63	J/molxK	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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1817749&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
ie:	Ionization energy
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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