1,1'-Biphenyl, 4,4'-dinitro-

Other names:	Biphenyl, 4,4'-dinitro-
	4,4'-Dinitrobiphenyl
	4,4'-Dinitrodiphenyl
	4,4'-Dinitrobifenyl
Inchi:	InChI=1S/C12H8N2O4/c15-13(16)11-5-1-9(2-6-11)10-3-7-12(8-4-10)14(17)18/h1-8H
InchiKey:	BDLNCFCZHNKBGI-UHFFFAOYSA-N
Formula:	C12H8N2O4
SMILES:	O=[N+]([O-])c1ccc(-c2ccc([N+](=O)[O-])cc2)cc1
Mol. weight [g/mol]:	244.20
CAS:	1528-74-1

Physical Properties

Property code	Value	Unit	Source
gf	326.82	kJ/mol	Joback Method
hf	137.59	kJ/mol	Joback Method
hfus	36.86	kJ/mol	Joback Method
hvap	81.36	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	3.170		Crippen Method
mcvol	167.260	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
tb	840.96	K	Joback Method
tc	1132.36	K	Joback Method
tf	590.10	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.48	J/mol×K	840.96	Joback Method
cpg	468.03	J/mol×K	889.53	Joback Method
cpg	477.38	J/mol×K	938.09	Joback Method
cpg	485.65	J/mol×K	986.66	Joback Method
cpg	492.96	J/mol×K	1035.23	Joback Method

cpg	499.43	J/mol×K	1083.80	Joback Method
cpg	505.17	J/mol×K	1132.36	Joback Method
hsubt	104.60 ± 1.80	kJ/mol	434.50	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=C1528741&Units=SI
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
gf:	Standard Gibbs free energy of formation
hf:	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