

1,1'-Biphenyl, 2,2'-dinitro-

Other names:	Biphenyl, 2,2'-dinitro- 2,2'-Dinitrobiphenyl 2,2'-Dinitrobiphenyl, 2,2'-dinitro- 2,2'-Dinitrodiphenyl
Inchi:	InChI=1S/C12H8N2O4/c15-13(16)11-7-3-1-5-9(11)10-6-2-4-8-12(10)14(17)18/h1-8H
InchiKey:	QAFJHDNFUMKVIE-UHFFFAOYSA-N
Formula:	C12H8N2O4
SMILES:	O=[N+]([O-])c1ccccc1-c1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	244.20
CAS:	2436-96-6

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
rinpol	349.40		NIST Webbook
rinpol	346.71		NIST Webbook
rinpol	346.71		NIST Webbook
rinpol	349.40		NIST Webbook
rinpol	345.99		NIST Webbook
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
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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

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2436966&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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