

1,1'-Biphenyl, 2,2'-dimethyl-6,6'-dinitro-

Other names:	2,2'-Dimethyl-6,6'-dinitro-diphenyl
Inchi:	InChI=1S/C14H12N2O4/c1-9-5-3-7-11(15(17)18)13(9)14-10(2)6-4-8-12(14)16(19)20/h3-
InchiKey:	UFWJYJCNLOWJCO-UHFFFAOYSA-N
Formula:	C14H12N2O4
SMILES:	<chem>Cc1cccc([N+](=O)[O-])c1-c1c(C)cccc1[N+](=O)[O-]</chem>
Mol. weight [g/mol]:	272.26
CAS:	55153-02-1

Physical Properties

Property code	Value	Unit	Source
gf	324.40	kJ/mol	Joback Method
hf	73.37	kJ/mol	Joback Method
hfus	41.26	kJ/mol	Joback Method
hvap	87.14	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	3.787		Crippen Method
mcvol	195.440	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
tb	896.68	K	Joback Method
tc	1175.16	K	Joback Method
tf	637.68	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.54	J/molxK	896.68	Joback Method
cpg	572.73	J/molxK	943.09	Joback Method
cpg	582.74	J/molxK	989.51	Joback Method
cpg	591.66	J/molxK	1035.92	Joback Method
cpg	599.56	J/molxK	1082.33	Joback Method
cpg	606.55	J/molxK	1128.75	Joback Method
cpg	612.71	J/molxK	1175.16	Joback Method

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=C55153021&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
hvp:	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

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