

2,2'-Dinitrobibenzyl

Other names:	Benzene, 1,1'-(1,2-ethanediyl)bis[2-nitro-Bibenzyl, 2,2'-dinitro-Dinitro-2,2' dibenzyl o,o'-dinitrobibenzyl
Inchi:	InChI=1S/C14H12N2O4/c17-15(18)13-7-3-1-5-11(13)9-10-12-6-2-4-8-14(12)16(19)20/h1
InchiKey:	YBOZRPPSBVIHGJ-UHFFFAOYSA-N
Formula:	C14H12N2O4
SMILES:	O=[N+]([O-])c1ccccc1CCc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	272.26
CAS:	16968-19-7

Physical Properties

Property code	Value	Unit	Source
gf	343.66	kJ/mol	Joback Method
hf	96.31	kJ/mol	Joback Method
hfus	42.04	kJ/mol	Joback Method
hvap	85.82	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	3.288		Crippen Method
mcvol	195.440	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
rinpol	372.85		NIST Webbook
rinpol	372.85		NIST Webbook
tb	886.72	K	Joback Method
tc	1163.96	K	Joback Method
tf	612.64	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.16	J/molxK	886.72	Joback Method
cpg	576.51	J/molxK	932.93	Joback Method
cpg	586.69	J/molxK	979.13	Joback Method

cpg	595.81	J/mol×K	1025.34	Joback Method
cpg	604.00	J/mol×K	1071.54	Joback Method
cpg	611.37	J/mol×K	1117.75	Joback Method
cpg	618.04	J/mol×K	1163.96	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=C16968197&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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