4,4'-Dinitrobibenzyl

Other names:	4,4'-Dinitrodibenzyl
	Benzene, 1,1'-(1,2-ethanediyl)bis[4-nitro-
	p,p'-Dinitrobibenzyl
	p,p'-Dinitrodibenzyl
	Bibenzyl, 4,4'-dinitro-
	1,2-Bis(p-nitrophenyl)ethane
	1,2-Bis(4-nitrophenyl)ethane
	1,2-Ethanediylbis(4-nitrobenzene)
	1,1'-(1,2-Ethanediyl)bis(4-nitrobenzene)
	NSC 60022
	NSC 608
Inchi:	InChI=1S/C14H12N2O4/c17-15(18)13-7-3-11(4-8-13)1-2-12-5-9-14(10-6-12)16(19)20/h3
InchiKey:	BSNKHEKTRWNNAC-UHFFFAOYSA-N
Formula:	C14H12N2O4
SMILES:	O=[N+]([O-])c1ccc(CCc2ccc([N+](=O)[O-])cc2)cc1
Mol. weight [g/mol]:	272.26
CAS:	736-30-1

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
ie	9.50 ± 0.10	eV	NIST Webbook
ie	9.77 ± 0.05	eV	NIST Webbook
log10ws	-5.19		Crippen Method
logp	3.288		Crippen Method
mcvol	195.440	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
rinpol	419.60		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/mol×K	886.72	Joback Method
cpg	576.51	J/mol×K	932.93	Joback Method
cpg	586.69	J/mol×K	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: 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=C736301&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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