1,3,5-Trinitro-2-[2-(2,4,6-trinitrophenyl)ethyl]benze

Other names: 2,2',4,4',6,6'-Hexanitrodibenzyl
Bibenzyl, 2,2',4,4',6,6'-hexanitro-
Benzene, 1,1'-(1,2-ethanediyl)bis[2,4,6-trinitro-
Inchi: InChI=1S/C14H8N6O12/c21-15(22)7-3-11(17(25)26)9(12(4-7)18(27)28)1-2-10-13(19(29)
InchiKey: VCAOQUOHRYQAPU-UHFFFAOYSA-N
Formula: C14H8N6O12
SMILES: O=[N+]([O-])c1cc([N+](=O)[O-])c(CCc2c([N+](=O)[O-])cc([N+](=O)[O-])cc2[N+](=O)[O-])c(
Mol. weight [g/mol]: 452.25
CAS: 5180-53-0

Physical Properties

Property code	Value	Unit	Source
chs	-6623.00 ± 3.00	kJ/mol	NIST Webbook
gf	447.34	kJ/mol	Joback Method
hf	7.39	kJ/mol	Joback Method
hfs	-30.00 ± 3.00	kJ/mol	NIST Webbook
hfus	85.93	kJ/mol	Joback Method
hvap	154.83	kJ/mol	Joback Method
log10ws	-7.79		Crippen Method
logp	2.921		Crippen Method
mcvol	265.120	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
tb	1514.00	K	Joback Method
tc	1856.39	K	Joback Method
tf	1237.16	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.29	J/mol×K	1514.00	Joback Method
cpg	802.79	J/mol×K	1571.07	Joback Method
cpg	802.03	J/mol×K	1628.13	Joback Method
cpg	801.21	J/mol×K	1685.20	Joback Method

cpg	800.52	J/mol×K	1742.26	Joback Method
cpg	800.16	J/mol×K	1799.33	Joback Method
cpg	800.33	J/mol×K	1856.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5180530&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume