2,2'-Dimethyl-4,4'-dinitrobibenzyl

Inchi: InChI=1S/C16H16N2O4/c1-11-9-15(17(19)20)7-5-13(11)3-4-14-6-8-16(18(21)22)10-12(1
InchiKey: DUSWUNUUPHBELH-UHFFFAOYSA-N
Formula: C16H16N2O4
SMILES: Cc1cc([N+](=O)[O-])ccc1CCc1ccc([N+](=O)[O-])cc1C
Mol. weight [g/mol]: 300.31
CAS: 87517-98-4

Physical Properties

Property code	Value	Unit	Source
gf	341.24	kJ/mol	Joback Method
hf	32.09	kJ/mol	Joback Method
hfus	46.44	kJ/mol	Joback Method
hvap	91.59	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	3.905		Crippen Method
mcvol	223.620	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
rinpol	452.39		NIST Webbook
rinpol	452.39		NIST Webbook
tb	942.44	K	Joback Method
tc	1209.60	K	Joback Method
tf	660.22	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	673.11	J/mol×K	942.44	Joback Method
cpg	684.83	J/mol×K	986.97	Joback Method
cpg	695.38	J/mol×K	1031.49	Joback Method
cpg	704.85	J/mol×K	1076.02	Joback Method
cpg	713.34	J/mol×K	1120.55	Joback Method
cpg	720.94	J/mol×K	1165.08	Joback Method
cpg	727.73	J/mol×K	1209.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87517984&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

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