Bis-(2,4,6-trichloro-3-nitro-5-methyl-benzene)

Inchi: InChI=1S/C14H6Cl6N2O4/c1-3-7(15)5(11(19)13(9(3)17)21(23)24)6-8(16)4(2)10(18)14(1
InchiKey: RKMYVKBGFHNXFA-UHFFFAOYSA-N
Formula: C14H6Cl6N2O4
SMILES: Cc1c(Cl)c(-c2c(Cl)c(C)c(Cl)c([N+](=O)[O-])c2Cl)c(Cl)c([N+](=O)[O-])c1Cl
Mol. weight [g/mol]: 478.93
CAS: 6950-45-4

Physical Properties

Property code	Value	Unit	Source
gf	195.04	kJ/mol	Joback Method
hf	-89.89	kJ/mol	Joback Method
hfus	64.11	kJ/mol	Joback Method
hvap	117.42	kJ/mol	Joback Method
log10ws	-10.44		Crippen Method
logp	7.707		Crippen Method
mcvol	268.880	ml/mol	McGowan Method
pc	1978.82	kPa	Joback Method
tb	1151.14	K	Joback Method
tc	1440.18	K	Joback Method
tf	892.32	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.07	J/mol×K	1151.14	Joback Method
cpg	637.47	J/mol×K	1199.31	Joback Method
cpg	639.82	J/mol×K	1247.49	Joback Method
cpg	641.16	J/mol×K	1295.66	Joback Method
cpg	641.53	J/mol×K	1343.83	Joback Method
cpg	640.94	J/mol×K	1392.01	Joback Method
cpg	639.45	J/mol×K	1440.18	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6950454&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume