2,2,2-Trichloro-n1,n1-bis(4-nitrophenyl)-1,1-ethan

Other names: 2,2,2-Trichloro-n<1>,n<1>-bis(4-nitrophenyl)-1,1-ethanediamine
Inchi: InChI=1S/C14H11Cl3N4O4/c15-14(16,17)13(18-9-1-5-11(6-2-9)20(22)23)19-10-3-7-12(8
InchiKey: WAIXKZLQJUGXPZ-UHFFFAOYSA-N
Formula: C14H11Cl3N4O4
SMILES: O=[N+]([O-])c1ccc(NC(Nc2ccc([N+](=O)[O-])cc2)C(Cl)(Cl)Cl)cc1
Mol. weight [g/mol]: 405.62
CAS: 39809-83-1

Physical Properties

Property code	Value	Unit	Source
gf	487.05	kJ/mol	Joback Method
hf	142.00	kJ/mol	Joback Method
hfus	53.89	kJ/mol	Joback Method
hvap	110.16	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	4.723		Crippen Method
mcvol	252.120	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
tb	1095.68	K	Joback Method
tc	1384.10	K	Joback Method
tf	795.14	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.49	J/mol×K	1095.68	Joback Method
cpg	716.08	J/mol×K	1143.75	Joback Method
cpg	723.33	J/mol×K	1191.82	Joback Method
cpg	730.46	J/mol×K	1239.89	Joback Method
cpg	737.67	J/mol×K	1287.96	Joback Method
cpg	745.16	J/mol×K	1336.03	Joback Method
cpg	753.16	J/mol×K	1384.10	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=C39809831&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
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