2,2,2-Trichloro-n,n'-bis(3,4-dichlorophenyl) ethylidene diamine

Inchi: InChI=1S/C14H9Cl7N2/c15-9-3-1-7(5-11(9)17)22-13(14(19,20)21)23-8-2-4-10(16)12(18)6-8/h1-6,13,22-23H

InchiKey: SRLLHBBTZZPDBN-UHFFFAOYSA-N

Formula: C14H9Cl7N2

SMILES: Clc1ccc(NC(Nc2ccc(Cl)c(Cl)c2)C(Cl)(Cl)Cl)cc1Cl

Mol. weight [g/mol]: 453.41

CAS: 53723-87-8

Physical Properties

Property code	Value	Unit	Source
gf	348.97	kJ/mol	Joback Method
hf	77.62	kJ/mol	Joback Method
hfus	47.18	kJ/mol	Joback Method
hvap	95.84	kJ/mol	Joback Method
log10ws	-8.05		Crippen Method
logp	7.521		Crippen Method
mcvol	266.240	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
tb	951.68	K	Joback Method
tc	1220.13	K	Joback Method
tf	652.64	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.83	J/mol×K	951.68	Joback Method
cpg	625.49	J/mol×K	996.42	Joback Method
cpg	632.49	J/mol×K	1041.16	Joback Method
cpg	638.99	J/mol×K	1085.91	Joback Method
cpg	645.11	J/mol×K	1130.65	Joback Method
cpg	651.00	J/mol×K	1175.39	Joback Method
cpg	656.80	J/mol×K	1220.13	Joback Method

Sources

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=C53723878&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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