

2,2,2-Trichloro-n,n'-bis(p-bromophenyl) ethylidene diamine

Inchi:	InChI=1S/C14H11Br2Cl3N2/c15-9-1-5-11(6-2-9)20-13(14(17,18)19)21-12-7-3-10(16)4-8
InchiKey:	LPTYLIBUBROVDY-UHFFFAOYSA-N
Formula:	C14H11Br2Cl3N2
SMILES:	<chem>C1C(Cl)(Cl)C(Nc1ccc(Br)cc1)Nc1ccc(Br)cc1</chem>
Mol. weight [g/mol]:	473.42
CAS:	83320-61-0

Physical Properties

Property code	Value	Unit	Source
gf	444.59	kJ/mol	Joback Method
hf	216.18	kJ/mol	Joback Method
hfus	41.74	kJ/mol	Joback Method
hvap	89.85	kJ/mol	Joback Method
log10ws	-7.63		Crippen Method
logp	6.432		Crippen Method
mcvol	252.280	ml/mol	McGowan Method
pc	2921.84	kPa	Joback Method
tb	924.32	K	Joback Method
tc	1202.56	K	Joback Method
tf	627.52	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.37	J/molxK	924.32	Joback Method
cpg	611.66	J/molxK	970.69	Joback Method
cpg	620.35	J/molxK	1017.07	Joback Method
cpg	628.65	J/molxK	1063.44	Joback Method
cpg	636.75	J/molxK	1109.81	Joback Method
cpg	644.87	J/molxK	1156.19	Joback Method
cpg	653.22	J/molxK	1202.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C83320610&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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