Alpha,alpha,alpha,2,4,5-hexachloroacetanilide

Inchi: InChI=1S/C8H3Cl6NO/c9-3-1-5(11)6(2-4(3)10)15-7(16)8(12,13)14/h1-2H,(H,15,16)
InchiKey: KTEQMHWNTSFTSS-UHFFFAOYSA-N
Formula: C8H3Cl6NO
SMILES: O=C(Nc1cc(Cl)c(Cl)cc1Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 341.83
CAS: 33560-57-5

Physical Properties

Property code	Value	Unit	Source
gf	-8.27	kJ/mol	Joback Method
hf	-168.63	kJ/mol	Joback Method
hfus	33.82	kJ/mol	Joback Method
hvap	75.86	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.956		Crippen Method
mcvol	184.810	ml/mol	McGowan Method
pc	2995.87	kPa	Joback Method
tb	749.45	K	Joback Method
tc	1008.70	K	Joback Method
tf	528.43	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.72	J/mol×K	749.45	Joback Method
cpg	360.70	J/mol×K	792.66	Joback Method
cpg	366.00	J/mol×K	835.87	Joback Method
cpg	370.71	J/mol×K	879.08	Joback Method
cpg	374.91	J/mol×K	922.28	Joback Method
cpg	378.67	J/mol×K	965.49	Joback Method
cpg	382.07	J/mol×K	1008.70	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=C33560575&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