2,2,2',4',5'-Pentachloroacetanilide

Inchi: InChI=1S/C8H4Cl5NO/c9-3-1-5(11)6(2-4(3)10)14-8(15)7(12)13/h1-2,7H,(H,14,15)
InchiKey: XAZSAUSDMZJMSS-UHFFFAOYSA-N
Formula: C8H4Cl5NO
SMILES: O=C(Nc1cc(Cl)c(Cl)cc1Cl)C(Cl)Cl
Mol. weight [g/mol]: 307.39
CAS: 33560-51-9

Physical Properties

Property code	Value	Unit	Source
gf	-1.62	kJ/mol	Joback Method
hf	-149.42	kJ/mol	Joback Method
hfus	33.51	kJ/mol	Joback Method
hvap	72.38	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.389		Crippen Method
mcvol	172.570	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
tb	714.81	K	Joback Method
tc	962.64	K	Joback Method
tf	481.09	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.57	J/mol×K	714.81	Joback Method
cpg	342.66	J/mol×K	756.12	Joback Method
cpg	349.09	J/mol×K	797.42	Joback Method
cpg	354.89	J/mol×K	838.73	Joback Method
cpg	360.11	J/mol×K	880.03	Joback Method
cpg	364.76	J/mol×K	921.34	Joback Method
cpg	368.89	J/mol×K	962.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33560519&Units=SI
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

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