2,2',4',5'-Tetrachloroacetanilide

Other names:	Acetamide, 2-chloro-N-(2,4,5-trichlorophenyl)- Acetanilide, 2,2',4',5'-tetrachloro- 2',4',6'-Trichloro-2-chloroacetanilide
Inchi:	InChI=1S/C8H5Cl4NO/c9-3-8(14)13-7-2-5(11)4(10)1-6(7)12/h1-2H,3H2,(H,13,14)
InchiKey:	GQRWKOPRUXSOBA-UHFFFAOYSA-N
Formula:	C8H5Cl4NO
SMILES:	O=C(CCl)Nc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	272.94
CAS:	23595-42-8

Physical Properties

Property code	Value	Unit	Source
gf	12.75	kJ/mol	Joback Method
hf	-128.40	kJ/mol	Joback Method
hfus	32.84	kJ/mol	Joback Method
hvap	68.39	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.824		Crippen Method
mcvol	160.330	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
tb	677.82	K	Joback Method
tc	918.30	K	Joback Method
tf	466.17	K	Joback Method
vc	0.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.01	J/mol×K	677.82	Joback Method
cpg	324.81	J/mol×K	717.90	Joback Method
cpg	331.98	J/mol×K	757.98	Joback Method
cpg	338.55	J/mol×K	798.06	Joback Method
cpg	344.53	J/mol×K	838.14	Joback Method
cpg	349.97	J/mol×K	878.22	Joback Method

cpg	354.89	J/mol×K	918.30	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23595428&Units=SI

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