

Alpha,alpha,alpha,m-tetrachloroacetanilide

Inchi:	InChI=1S/C8H5Cl4NO/c9-5-2-1-3-6(4-5)13-7(14)8(10,11)12/h1-4H,(H,13,14)
InchiKey:	ZCNFWVGKVHRKCD-UHFFFAOYSA-N
Formula:	C8H5Cl4NO
SMILES:	O=C(Nc1cccc(Cl)c1)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	272.94
CAS:	3004-73-7

Physical Properties

Property code	Value	Unit	Source
gf	34.85	kJ/mol	Joback Method
hf	-114.21	kJ/mol	Joback Method
hfus	26.20	kJ/mol	Joback Method
hvap	65.77	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.649		Crippen Method
mcvol	160.330	ml/mol	McGowan Method
pc	3368.44	kPa	Joback Method
tb	664.63	K	Joback Method
tc	918.20	K	Joback Method
tf	443.55	K	Joback Method
vc	0.602	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.54	J/mol×K	664.63	Joback Method
cpg	332.85	J/mol×K	706.89	Joback Method
cpg	340.28	J/mol×K	749.15	Joback Method
cpg	346.91	J/mol×K	791.41	Joback Method
cpg	352.83	J/mol×K	833.67	Joback Method
cpg	358.13	J/mol×K	875.94	Joback Method
cpg	362.90	J/mol×K	918.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3004737&Units=SI&Mask=3FFF
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

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

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