

2,3,3,3'-Tetrachloroacrylanilide

Inchi:	InChI=1S/C9H5Cl4NO/c10-5-2-1-3-6(4-5)14-9(15)7(11)8(12)13/h1-4H,(H,14,15)
InchiKey:	HLVCGIROEHDIQK-UHFFFAOYSA-N
Formula:	C9H5Cl4NO
SMILES:	O=C(Nc1cccc(Cl)c1)C(Cl)=C(Cl)Cl
Mol. weight [g/mol]:	284.95
CAS:	949-53-1

Physical Properties

Property code	Value	Unit	Source
gf	103.55	kJ/mol	Joback Method
hf	-28.46	kJ/mol	Joback Method
hfus	33.79	kJ/mol	Joback Method
hvap	69.41	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.164		Crippen Method
mcvol	170.120	ml/mol	McGowan Method
pc	3170.40	kPa	Joback Method
tb	694.66	K	Joback Method
tc	946.73	K	Joback Method
tf	419.40	K	Joback Method
vc	0.650	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.87	J/molxK	694.66	Joback Method
cpg	352.21	J/molxK	736.67	Joback Method
cpg	359.76	J/molxK	778.68	Joback Method
cpg	366.61	J/molxK	820.69	Joback Method
cpg	372.85	J/molxK	862.71	Joback Method
cpg	378.56	J/molxK	904.72	Joback Method
cpg	383.81	J/molxK	946.73	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=C949531&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

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