2,2,3',4'-Tetrachloropropionanilide

Inchi: InChI=1S/C9H7Cl4NO/c1-9(12,13)8(15)14-5-2-3-6(10)7(11)4-5/h2-4H,1H3,(H,14,15)

InchiKey: YGRDEBCXIKCCIA-UHFFFAOYSA-N

Formula: C9H7Cl4NO

SMILES: CC(Cl)(Cl)C(=O)Nc1ccc(Cl)c(Cl)c1

Mol. weight [g/mol]: 286.97

CAS: 37995-08-7

Physical Properties

Property code	Value	Unit	Source
gf	33.64	kJ/mol	Joback Method
hf	-146.32	kJ/mol	Joback Method
hfus	28.40	kJ/mol	Joback Method
hvap	68.65	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	4.126		Crippen Method
mcvol	174.420	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
tb	692.49	K	Joback Method
tc	941.20	K	Joback Method
tf	467.34	K	Joback Method
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.85	J/mol×K	692.49	Joback Method
cpg	378.83	J/mol×K	733.94	Joback Method
cpg	386.95	J/mol×K	775.39	Joback Method
cpg	394.31	J/mol×K	816.85	Joback Method
cpg	400.96	J/mol×K	858.30	Joback Method
cpg	406.99	J/mol×K	899.75	Joback Method
cpg	412.49	J/mol×K	941.20	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=C37995087&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