2,2,2',4'-Tetrachloropropionanilide

Inchi: InChI=1S/C9H7Cl4NO/c1-9(12,13)8(15)14-7-3-2-5(10)4-6(7)11/h2-4H,1H3,(H,14,15)
InchiKey: LYLOVGGYRYQRNQ-UHFFFAOYSA-N
Formula: C9H7Cl4NO
SMILES: CC(Cl)(Cl)C(=O)Nc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 286.97
CAS: 56511-20-7

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=C56511207&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

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