2',4',5'-TRICHLOROACETANILIDE

Other names:	2,4,5-Trichloroacetanilide
	Acetamide, N-(2,4,5-trichlorophenyl)-
	N-(2,4,5-trichlorophenyl)acetamide
Inchi:	InChI=1S/C8H6Cl3NO/c1-4(13)12-8-3-6(10)5(9)2-7(8)11/h2-3H,1H3,(H,12,13)
InchiKey:	VUSLTUGEJURGLB-UHFFFAOYSA-N
Formula:	C8H6Cl3NO
SMILES:	CC(=O)Nc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	238.50

Physical Properties

Property code	Value	Unit	Source
hfus	28.64	kJ/mol	Joback Method
ie	8.29	eV	Cheméo Relay (1.0)
log10ws	-3.62		Cheméo Relay (1.0)
logp	3.605		Crippen Method
mcvol	148.090	ml/mol	McGowan Method
tb	560.54	K	Cheméo Relay (1.0)
tf	380.42	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.89	J/mol×K	640.39	Joback Method
cpg	306.55	J/mol×K	680.00	Joback Method
cpg	314.57	J/mol×K	719.62	Joback Method
cpg	321.98	J/mol×K	759.23	Joback Method
cpg	328.79	J/mol×K	798.85	Joback Method
cpg	335.04	J/mol×K	838.46	Joback Method
cpg	340.74	J/mol×K	878.08	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23627249&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point