2',4'-Dichloroacetanilide

Other names: Acetanilide, 2',4'-dichloro-
2,4-Dichloroacetanilide
2',4'-Dichloroacetanilide
Inchi: InChI=1S/C8H7Cl2NO/c1-5(12)11-8-3-2-6(9)4-7(8)10/h2-4H,1H3,(H,11,12)
InchiKey: GZSGTFDLLISMMA-UHFFFAOYSA-N
Formula: C8H7Cl2NO
SMILES: CC(=O)Nc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 204.06

Physical Properties

Property code	Value	Unit	Source
hf	-193.31	kJ/mol	Cheméo Relay (1.0)
hfus	24.83	kJ/mol	Joback Method
hvap	76.18	kJ/mol	Cheméo Relay (1.0)
ie	8.09 ± 0.03	eV	NIST Webbook
log10ws	-2.83		Cheméo Relay (1.0)
logp	2.952		Crippen Method
mcvol	135.850	ml/mol	McGowan Method
tb	550.33	K	Cheméo Relay (1.0)
tf	356.96	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.93	J/mol×K	597.98	Joback Method
cpg	288.66	J/mol×K	636.89	Joback Method
cpg	297.69	J/mol×K	675.80	Joback Method
cpg	306.07	J/mol×K	714.71	Joback Method
cpg	313.81	J/mol×K	753.62	Joback Method
cpg	320.94	J/mol×K	792.53	Joback Method
cpg	327.50	J/mol×K	831.44	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6975297&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization 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