3',4'-Dichlorophenylacetanilide

Inchi: InChI=1S/C14H11Cl2NO/c15-12-7-6-11(9-13(12)16)17-14(18)8-10-4-2-1-3-5-10/h1-7,9H
InchiKey: WOLDJAKASQLODM-UHFFFAOYSA-N
Formula: C14H11Cl2NO
SMILES: O=C(Cc1ccccc1)Nc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 280.15
CAS: 27816-82-6

Physical Properties

Property code	Value	Unit	Source
gf	209.17	kJ/mol	Joback Method
hf	27.24	kJ/mol	Joback Method
hfus	34.41	kJ/mol	Joback Method
hvap	74.59	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.175		Crippen Method
mcvol	196.630	ml/mol	McGowan Method
pc	2690.21	kPa	Joback Method
tb	761.94	K	Joback Method
tc	1011.67	K	Joback Method
tf	487.85	K	Joback Method
vc	0.743	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.46	J/mol×K	761.94	Joback Method
cpg	497.48	J/mol×K	803.56	Joback Method
cpg	508.43	J/mol×K	845.18	Joback Method
cpg	518.37	J/mol×K	886.80	Joback Method
cpg	527.38	J/mol×K	928.43	Joback Method
cpg	535.54	J/mol×K	970.05	Joback Method
cpg	542.92	J/mol×K	1011.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27816826&Units=SI
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

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