2-Chloropropionanilide

Other names: Propanamide,N-(2-chlorophenyl)-
Inchi: InChI=1S/C9H10ClNO/c1-2-9(12)11-8-6-4-3-5-7(8)10/h3-6H,2H2,1H3,(H,11,12)
InchiKey: VCVUMBWLSGNGFA-UHFFFAOYSA-N
Formula: C9H10ClNO
SMILES: CCC(=O)Nc1ccccc1Cl
Mol. weight [g/mol]: 183.63
CAS: 2760-32-9

Physical Properties

Property code	Value	Unit	Source
gf	76.22	kJ/mol	Joback Method
hf	-78.88	kJ/mol	Joback Method
hfus	23.61	kJ/mol	Joback Method
hvap	56.13	kJ/mol	Joback Method
ie	8.45 ± 0.05	eV	NIST Webbook
log10ws	-2.78		Crippen Method
logp	2.688		Crippen Method
mcvol	137.700	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
tb	578.45	K	Joback Method
tc	802.68	K	Joback Method
tf	362.64	K	Joback Method
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.69	J/mol×K	578.45	Joback Method
cpg	314.51	J/mol×K	615.82	Joback Method
cpg	325.54	J/mol×K	653.19	Joback Method
cpg	335.82	J/mol×K	690.57	Joback Method
cpg	345.37	J/mol×K	727.94	Joback Method
cpg	354.23	J/mol×K	765.31	Joback Method
cpg	362.44	J/mol×K	802.68	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=C2760329&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
ie:	Ionization energy
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