Hexanamide, N-(3-chlorophenyl)-

Inchi: InChI=1S/C12H16ClNO/c1-2-3-4-8-12(15)14-11-7-5-6-10(13)9-11/h5-7,9H,2-4,8H2,1H3,(

InchiKey: BAUYPJBSRHYPFK-UHFFFAOYSA-N

Formula: C12H16ClNO

SMILES: CCCCCC(O)=Nc1cccc(Cl)c1

Mol. weight [g/mol]: 225.72

Physical Properties

Property code	Value	Unit	Source
hf	-161.49	kJ/mol	Joback Method
hvap	69.70	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	4.508		Crippen Method
mcvol	179.970	ml/mol	McGowan Method
pc	2269.73	kPa	Joback Method
rinpol	1916.00		NIST Webbook
rinpol	1916.00		NIST Webbook
tb	711.79	K	Joback Method
tc	920.97	K	Joback Method

Sources

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=U307288&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: Enthalpy of formation 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature