Pentanamide, N-(3-methylphenyl)-5-chloro-

Inchi: InChI=1S/C12H16ClNO/c1-10-5-4-6-11(9-10)14-12(15)7-2-3-8-13/h4-6,9H,2-3,7-8H2,1H
InchiKey: KXBWQDPILGCNTC-UHFFFAOYSA-N
Formula: C12H16ClNO
SMILES: Cc1cccc(N=C(O)CCCCCl)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	-3.74		Crippen Method
logp	3.992		Crippen Method
mcvol	179.970	ml/mol	McGowan Method
pc	2269.73	kPa	Joback Method
rinpol	1973.00		NIST Webbook
rinpol	1973.00		NIST Webbook
tb	711.79	K	Joback Method
tc	920.97	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U307359&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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