Butanamide, N-(3-chlorophenyl)-

Inchi: InChI=1S/C10H12ClNO/c1-2-4-10(13)12-9-6-3-5-8(11)7-9/h3,5-7H,2,4H2,1H3,(H,12,13)
InchiKey: QOKSOJARIYYAAO-UHFFFAOYSA-N
Formula: C10H12ClNO
SMILES: CCCC(O)=Nc1cccc(Cl)c1
Mol. weight [g/mol]: 197.66

Physical Properties

Property code	Value	Unit	Source
hf	-120.21	kJ/mol	Joback Method
hvap	65.25	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.728		Crippen Method
mcvol	151.790	ml/mol	McGowan Method
pc	2749.78	kPa	Joback Method
rinpol	1706.00		NIST Webbook
rinpol	1706.00		NIST Webbook
tb	666.03	K	Joback Method
tc	881.46	K	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=U306914&Units=SI

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