Pentanamide, N-(3-chlorophenyl)-

Inchi: InChI=1S/C11H14ClNO/c1-2-3-7-11(14)13-10-6-4-5-9(12)8-10/h4-6,8H,2-3,7H2,1H3,(H,1
InchiKey: LOQKNLXBLMIZPG-UHFFFAOYSA-N
Formula: C11H14ClNO
SMILES: CCCCC(=O)Nc1cccc(Cl)c1
Mol. weight [g/mol]: 211.69

Physical Properties

Property code	Value	Unit	Source
gf	93.06	kJ/mol	Joback Method
hf	-120.16	kJ/mol	Joback Method
hfus	28.79	kJ/mol	Joback Method
hvap	60.59	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.469		Crippen Method
mcvol	165.880	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
rinpol	1817.00		NIST Webbook
tb	624.21	K	Joback Method
tc	840.51	K	Joback Method
tf	385.18	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.23	J/mol×K	624.21	Joback Method
cpg	410.59	J/mol×K	660.26	Joback Method
cpg	423.10	J/mol×K	696.31	Joback Method
cpg	434.78	J/mol×K	732.36	Joback Method
cpg	445.68	J/mol×K	768.41	Joback Method
cpg	455.83	J/mol×K	804.46	Joback Method
cpg	465.27	J/mol×K	840.51	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=U306892&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
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
tf:	Normal melting (fusion) point
vc:	Critical Volume