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

Inchi: InChI=1S/C11H13Cl2NO/c12-7-2-1-6-11(15)14-10-5-3-4-9(13)8-10/h3-5,8H,1-2,6-7H2,(H
InchiKey: GYILROAJGQKZID-UHFFFAOYSA-N
Formula: C11H13Cl2NO
SMILES: O=C(CCCCCl)Nc1cccc(Cl)c1
Mol. weight [g/mol]: 246.13

Physical Properties

Property code	Value	Unit	Source
gf	81.13	kJ/mol	Joback Method
hf	-135.90	kJ/mol	Joback Method
hfus	32.99	kJ/mol	Joback Method
hvap	64.97	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.688		Crippen Method
mcvol	178.120	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
rinpol	2095.00		NIST Webbook
tb	661.64	K	Joback Method
tc	881.30	K	Joback Method
tf	415.10	K	Joback Method
vc	0.682	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.14	J/mol×K	661.64	Joback Method
cpg	434.49	J/mol×K	698.25	Joback Method
cpg	445.99	J/mol×K	734.86	Joback Method
cpg	456.68	J/mol×K	771.47	Joback Method
cpg	466.60	J/mol×K	808.08	Joback Method
cpg	475.80	J/mol×K	844.69	Joback Method
cpg	484.32	J/mol×K	881.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307360&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

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