Pentanamide, N-(4-fluorophenyl)-5-chloro-

Inchi: InChI=1S/C11H13ClFNO/c12-8-2-1-3-11(15)14-10-6-4-9(13)5-7-10/h4-7H,1-3,8H2,(H,14
InchiKey: RBNLFAFIPVALBL-UHFFFAOYSA-N
Formula: C11H13ClFNO
SMILES: O=C(CCCCCl)Nc1ccc(F)cc1
Mol. weight [g/mol]: 229.68

Physical Properties

Property code	Value	Unit	Source
gf	-101.75	kJ/mol	Joback Method
hf	-316.27	kJ/mol	Joback Method
hfus	31.87	kJ/mol	Joback Method
hvap	59.77	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.173		Crippen Method
mcvol	167.650	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
rinpol	1880.00		NIST Webbook
tb	623.48	K	Joback Method
tc	830.13	K	Joback Method
tf	385.77	K	Joback Method
vc	0.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.37	J/mol×K	623.48	Joback Method
cpg	418.09	J/mol×K	657.92	Joback Method
cpg	430.01	J/mol×K	692.36	Joback Method
cpg	441.17	J/mol×K	726.80	Joback Method
cpg	451.60	J/mol×K	761.25	Joback Method
cpg	461.32	J/mol×K	795.69	Joback Method
cpg	470.39	J/mol×K	830.13	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=U307358&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