Propanamide, N-(4-fluorophenyl)-3-chloro-

Inchi: InChI=1S/C9H9ClFNO/c10-6-5-9(13)12-8-3-1-7(11)2-4-8/h1-4H,5-6H2,(H,12,13)
InchiKey: WXMWLNAPEHYULF-UHFFFAOYSA-N
Formula: C9H9ClFNO
SMILES: O=C(CCCl)Nc1ccc(F)cc1
Mol. weight [g/mol]: 201.62

Physical Properties

Property code	Value	Unit	Source
gf	-118.59	kJ/mol	Joback Method
hf	-274.99	kJ/mol	Joback Method
hfus	26.69	kJ/mol	Joback Method
hvap	55.32	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.393		Crippen Method
mcvol	139.470	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
rinpol	1647.00		NIST Webbook
rinpol	1647.00		NIST Webbook
tb	577.72	K	Joback Method
tc	791.12	K	Joback Method
tf	363.23	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.95	J/mol×K	577.72	Joback Method
cpg	322.17	J/mol×K	613.29	Joback Method
cpg	332.66	J/mol×K	648.85	Joback Method
cpg	342.44	J/mol×K	684.42	Joback Method
cpg	351.56	J/mol×K	719.99	Joback Method
cpg	360.03	J/mol×K	755.56	Joback Method
cpg	367.89	J/mol×K	791.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307225&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

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