Propanamide, N-(2-fluorophenyl)-2-chloro-

Inchi: InChI=1S/C9H9ClFNO/c1-6(10)9(13)12-8-5-3-2-4-7(8)11/h2-6H,1H3,(H,12,13)
InchiKey: SCIHVRDPCNXWQL-UHFFFAOYSA-N
Formula: C9H9ClFNO
SMILES: CC(Cl)C(=O)Nc1ccccc1F
Mol. weight [g/mol]: 201.62

Physical Properties

Property code	Value	Unit	Source
gf	-121.03	kJ/mol	Joback Method
hf	-280.27	kJ/mol	Joback Method
hfus	23.17	kJ/mol	Joback Method
hvap	54.93	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.391		Crippen Method
mcvol	139.470	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
rinpol	1398.00		NIST Webbook
tb	577.28	K	Joback Method
tc	795.26	K	Joback Method
tf	348.23	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.38	J/mol×K	577.28	Joback Method
cpg	322.90	J/mol×K	613.61	Joback Method
cpg	333.64	J/mol×K	649.94	Joback Method
cpg	343.65	J/mol×K	686.27	Joback Method
cpg	352.94	J/mol×K	722.60	Joback Method
cpg	361.55	J/mol×K	758.93	Joback Method
cpg	369.52	J/mol×K	795.26	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=U308382&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