Acetamide, N-(4-fluorophenyl)-2-chloro-

Inchi: InChI=1S/C8H7ClFNO/c9-5-8(12)11-7-3-1-6(10)2-4-7/h1-4H,5H2,(H,11,12)
InchiKey: JDAWWCJBFPBHFL-UHFFFAOYSA-N
Formula: C8H7ClFNO
SMILES: O=C(CCl)Nc1ccc(F)cc1
Mol. weight [g/mol]: 187.60

Physical Properties

Property code	Value	Unit	Source
gf	-127.01	kJ/mol	Joback Method
hf	-254.35	kJ/mol	Joback Method
hfus	24.10	kJ/mol	Joback Method
hvap	53.09	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.003		Crippen Method
mcvol	125.380	ml/mol	McGowan Method
pc	3560.02	kPa	Joback Method
rinpol	1417.00		NIST Webbook
tb	554.84	K	Joback Method
tc	771.92	K	Joback Method
tf	351.96	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.25	J/mol×K	554.84	Joback Method
cpg	276.54	J/mol×K	591.02	Joback Method
cpg	286.15	J/mol×K	627.20	Joback Method
cpg	295.09	J/mol×K	663.38	Joback Method
cpg	303.40	J/mol×K	699.56	Joback Method
cpg	311.11	J/mol×K	735.74	Joback Method
cpg	318.24	J/mol×K	771.92	Joback Method

Sources

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=U307235&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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