Acetamide, N-(2-fluorophenyl)-

Other names: 2'-Fluoroacetanilide
N-(2-fluorophenyl)acetamide
Inchi: InChI=1S/C8H8FNO/c1-6(11)10-8-5-3-2-4-7(8)9/h2-5H,1H3,(H,10,11)
InchiKey: AUZPZBPZWHEIDY-UHFFFAOYSA-N
Formula: C8H8FNO
SMILES: CC(=O)Nc1ccccc1F
Mol. weight [g/mol]: 153.15
CAS: 399-31-5

Physical Properties

Property code	Value	Unit	Source
gf	-115.08	kJ/mol	Joback Method
hf	-238.61	kJ/mol	Joback Method
hfus	19.91	kJ/mol	Joback Method
hvap	48.70	kJ/mol	Joback Method
ie	8.65	eV	NIST Webbook
ie	8.27 ± 0.03	eV	NIST Webbook
log10ws	-2.01		Crippen Method
logp	1.784		Crippen Method
mcvol	113.140	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
tb	517.41	K	Joback Method
tc	729.82	K	Joback Method
tf	322.04	K	Joback Method
vc	0.434	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.65	J/mol×K	517.41	Joback Method
cpg	253.72	J/mol×K	552.81	Joback Method
cpg	264.12	J/mol×K	588.21	Joback Method
cpg	273.86	J/mol×K	623.61	Joback Method
cpg	282.97	J/mol×K	659.01	Joback Method

cpg	291.48	J/mol×K	694.41	Joback Method
cpg	299.41	J/mol×K	729.82	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	414.20	K	1.90	NIST Webbook
tbrp	414.00 ± 1.00	K	1.90	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C399315&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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume