(2-fluorophenyl)urea

Inchi: InChI=1S/C7H7FN2O/c8-5-3-1-2-4-6(5)10-7(9)11/h1-4H,(H3,9,10,11)
InchiKey: PAWVOCWEWJXILY-UHFFFAOYSA-N
Formula: C7H7FN2O
SMILES: NC(=O)Nc1ccccc1F
Mol. weight [g/mol]: 154.14
CAS: 656-31-5

Physical Properties

Property code	Value	Unit	Source
gf	-57.05	kJ/mol	Joback Method
hf	-184.18	kJ/mol	Joback Method
hfus	22.51	kJ/mol	Joback Method
hvap	57.12	kJ/mol	Joback Method
ie	8.50	eV	NIST Webbook
log10ws	-2.00		Crippen Method
logp	1.316		Crippen Method
mcvol	109.030	ml/mol	McGowan Method
pc	4528.58	kPa	Joback Method
tb	567.06	K	Joback Method
tc	792.48	K	Joback Method
tf	394.03	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.98	J/mol×K	567.06	Joback Method
cpg	259.91	J/mol×K	604.63	Joback Method
cpg	269.15	J/mol×K	642.20	Joback Method
cpg	277.72	J/mol×K	679.77	Joback Method
cpg	285.65	J/mol×K	717.34	Joback Method
cpg	292.98	J/mol×K	754.91	Joback Method
cpg	299.72	J/mol×K	792.48	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=C656315&Units=SI&Mask=3FFF

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume