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

Other names: 4-Fluoroaniline, TFA
Inchi: InChI=1S/C8H5F4NO/c9-5-1-3-6(4-2-5)13-7(14)8(10,11)12/h1-4H,(H,13,14)
InchiKey: YTUKUMWAERJYPA-UHFFFAOYSA-N
Formula: C8H5F4NO
SMILES: O=C(Nc1ccc(F)cc1)C(F)(F)F
Mol. weight [g/mol]: 207.12

Physical Properties

Property code	Value	Unit	Source
gf	-696.67	kJ/mol	Joback Method
hf	-835.69	kJ/mol	Joback Method
hfus	21.73	kJ/mol	Joback Method
hvap	44.96	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.326		Crippen Method
mcvol	118.450	ml/mol	McGowan Method
pc	3246.73	kPa	Joback Method
rinpol	905.00		NIST Webbook
tb	511.99	K	Joback Method
tc	705.90	K	Joback Method
tf	326.23	K	Joback Method
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.19	J/mol×K	511.99	Joback Method
cpg	281.49	J/mol×K	544.31	Joback Method
cpg	291.05	J/mol×K	576.63	Joback Method
cpg	299.93	J/mol×K	608.95	Joback Method
cpg	308.15	J/mol×K	641.26	Joback Method
cpg	315.75	J/mol×K	673.58	Joback Method
cpg	322.77	J/mol×K	705.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307308&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
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