2-Butenamide, N-(4-fluorophenyl)-3-methyl-

Inchi: InChI=1S/C11H12FNO/c1-8(2)7-11(14)13-10-5-3-9(12)4-6-10/h3-7H,1-2H3,(H,13,14)
InchiKey: CHJVAINAJREZKY-UHFFFAOYSA-N
Formula: C11H12FNO
SMILES: CC(C)=CC(=O)Nc1ccc(F)cc1
Mol. weight [g/mol]: 193.22

Physical Properties

Property code	Value	Unit	Source
gf	-18.15	kJ/mol	Joback Method
hf	-193.10	kJ/mol	Joback Method
hfus	26.57	kJ/mol	Joback Method
hvap	55.42	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.730		Crippen Method
mcvol	151.110	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	1635.00		NIST Webbook
tb	590.09	K	Joback Method
tc	805.17	K	Joback Method
tf	336.81	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.62	J/mol×K	590.09	Joback Method
cpg	371.88	J/mol×K	625.94	Joback Method
cpg	384.27	J/mol×K	661.78	Joback Method
cpg	395.84	J/mol×K	697.63	Joback Method
cpg	406.64	J/mol×K	733.47	Joback Method
cpg	416.70	J/mol×K	769.32	Joback Method
cpg	426.09	J/mol×K	805.17	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=U307267&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