Butanamide, N-(4-fluorophenyl)-

Inchi: InChI=1S/C10H12FNO/c1-2-3-10(13)12-9-6-4-8(11)5-7-9/h4-7H,2-3H2,1H3,(H,12,13)
InchiKey: BIWQQFGZTRYRFG-UHFFFAOYSA-N
Formula: C10H12FNO
SMILES: CCCC(=O)Nc1ccc(F)cc1
Mol. weight [g/mol]: 181.21

Physical Properties

Property code	Value	Unit	Source
gf	-98.24	kJ/mol	Joback Method
hf	-279.89	kJ/mol	Joback Method
hfus	25.09	kJ/mol	Joback Method
hvap	53.16	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.564		Crippen Method
mcvol	141.320	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
rinpol	1508.00		NIST Webbook
rinpol	1508.00		NIST Webbook
tb	563.17	K	Joback Method
tc	768.98	K	Joback Method
tf	344.58	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.76	J/mol×K	563.17	Joback Method
cpg	344.67	J/mol×K	597.47	Joback Method
cpg	356.81	J/mol×K	631.77	Joback Method
cpg	368.22	J/mol×K	666.08	Joback Method
cpg	378.92	J/mol×K	700.38	Joback Method
cpg	388.94	J/mol×K	734.68	Joback Method
cpg	398.32	J/mol×K	768.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U306912&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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