Propanamide, N-(4-fluorophenyl)-2-methyl-

Inchi: InChI=1S/C10H12FNO/c1-7(2)10(13)12-9-5-3-8(11)4-6-9/h3-7H,1-2H3,(H,12,13)
InchiKey: XYITWGGFWSDVMU-UHFFFAOYSA-N
Formula: C10H12FNO
SMILES: CC(C)C(=O)Nc1ccc(F)cc1
Mol. weight [g/mol]: 181.21

Physical Properties

Property code	Value	Unit	Source
gf	-100.68	kJ/mol	Joback Method
hf	-285.17	kJ/mol	Joback Method
hfus	21.56	kJ/mol	Joback Method
hvap	52.77	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.420		Crippen Method
mcvol	141.320	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
rinpol	1446.00		NIST Webbook
tb	562.73	K	Joback Method
tc	772.92	K	Joback Method
tf	329.58	K	Joback Method
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.14	J/mol×K	562.73	Joback Method
cpg	345.38	J/mol×K	597.76	Joback Method
cpg	357.81	J/mol×K	632.79	Joback Method
cpg	369.47	J/mol×K	667.82	Joback Method
cpg	380.39	J/mol×K	702.85	Joback Method
cpg	390.59	J/mol×K	737.88	Joback Method
cpg	400.11	J/mol×K	772.92	Joback Method

Sources

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=U307319&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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