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

Inchi: InChI=1S/C11H14FNO/c1-11(2,3)10(14)13-9-6-4-8(12)5-7-9/h4-7H,1-3H3,(H,13,14)
InchiKey: DDRGTIBAQBROSP-UHFFFAOYSA-N
Formula: C11H14FNO
SMILES: CC(C)(C)C(=O)Nc1ccc(F)cc1
Mol. weight [g/mol]: 195.23

Physical Properties

Property code	Value	Unit	Source
gf	-86.98	kJ/mol	Joback Method
hf	-309.28	kJ/mol	Joback Method
hfus	20.26	kJ/mol	Joback Method
hvap	54.09	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.810		Crippen Method
mcvol	155.410	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
rinpol	1445.00		NIST Webbook
rinpol	1445.00		NIST Webbook
tb	582.82	K	Joback Method
tc	797.66	K	Joback Method
tf	358.27	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.33	J/mol×K	582.82	Joback Method
cpg	396.75	J/mol×K	618.63	Joback Method
cpg	410.18	J/mol×K	654.43	Joback Method
cpg	422.67	J/mol×K	690.24	Joback Method
cpg	434.27	J/mol×K	726.05	Joback Method
cpg	445.05	J/mol×K	761.85	Joback Method
cpg	455.06	J/mol×K	797.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307194&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