Propanamide, N-(4-fluorophenyl)-3-phenyl-

Inchi: InChI=1S/C15H14FNO/c16-13-7-9-14(10-8-13)17-15(18)11-6-12-4-2-1-3-5-12/h1-5,7-10
InchiKey: OIWMUPBNVSEYPP-UHFFFAOYSA-N
Formula: C15H14FNO
SMILES: O=C(CCc1ccccc1)Nc1ccc(F)cc1
Mol. weight [g/mol]: 243.28

Physical Properties

Property code	Value	Unit	Source
gf	56.27	kJ/mol	Joback Method
hf	-146.56	kJ/mol	Joback Method
hfus	32.08	kJ/mol	Joback Method
hvap	66.56	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.397		Crippen Method
mcvol	188.010	ml/mol	McGowan Method
pc	2550.76	kPa	Joback Method
rinpol	2069.00		NIST Webbook
rinpol	2069.00		NIST Webbook
tb	704.25	K	Joback Method
tc	933.27	K	Joback Method
tf	427.35	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.89	J/mol×K	704.25	Joback Method
cpg	514.39	J/mol×K	742.42	Joback Method
cpg	527.76	J/mol×K	780.59	Joback Method
cpg	540.07	J/mol×K	818.76	Joback Method
cpg	551.38	J/mol×K	856.93	Joback Method
cpg	561.77	J/mol×K	895.10	Joback Method
cpg	571.30	J/mol×K	933.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308114&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