

Pentanamide, N-(2-fluorophenyl)-

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C11H14FNO/c1-2-3-8-11(14)13-10-7-5-4-6-9(10)12/h4-7H,2-3,8H2,1H3,(H,13,

ZICWAPAXFADNMC-UHFFFAOYSA-N

C11H14FNO

CCCCC(=O)Nc1ccccc1F

195.23

Physical Properties

Property code	Value	Unit	Source
gf	-89.82	kJ/mol	Joback Method
hf	-300.53	kJ/mol	Joback Method
hfus	27.68	kJ/mol	Joback Method
hvap	55.38	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.954		Crippen Method
mcvol	155.410	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
rinpol	1519.00		NIST Webbook
tb	586.05	K	Joback Method
tc	788.78	K	Joback Method
tf	355.85	K	Joback Method
vc	0.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.93	J/mol×K	586.05	Joback Method
cpg	392.58	J/mol×K	619.84	Joback Method
cpg	405.43	J/mol×K	653.63	Joback Method
cpg	417.51	J/mol×K	687.41	Joback Method
cpg	428.86	J/mol×K	721.20	Joback Method
cpg	439.50	J/mol×K	754.99	Joback Method
cpg	449.46	J/mol×K	788.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308177&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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