Hexanamide, N-(4-fluorophenyl)-

Inchi: InChI=1S/C12H16FNO/c1-2-3-4-5-12(15)14-11-8-6-10(13)7-9-11/h6-9H,2-5H2,1H3,(H,14
InchiKey: WVQWWEIOTUTFQM-UHFFFAOYSA-N
Formula: C12H16FNO
SMILES: CCCCCC(=O)Nc1ccc(F)cc1
Mol. weight [g/mol]: 209.26

Physical Properties

Property code	Value	Unit	Source
gf	-81.40	kJ/mol	Joback Method
hf	-321.17	kJ/mol	Joback Method
hfus	30.27	kJ/mol	Joback Method
hvap	57.61	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.344		Crippen Method
mcvol	169.500	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
rinpol	1708.00		NIST Webbook
tb	608.93	K	Joback Method
tc	808.78	K	Joback Method
tf	367.12	K	Joback Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.71	J/mol×K	608.93	Joback Method
cpg	442.00	J/mol×K	642.24	Joback Method
cpg	455.46	J/mol×K	675.55	Joback Method
cpg	468.13	J/mol×K	708.86	Joback Method
cpg	480.04	J/mol×K	742.16	Joback Method
cpg	491.22	J/mol×K	775.47	Joback Method
cpg	501.69	J/mol×K	808.78	Joback Method

Sources

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=U307286&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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