Cyclopentanecarboxamide, N-(2-fluorophenyl)-

Inchi: InChI=1S/C12H14FNO/c13-10-7-3-4-8-11(10)14-12(15)9-5-1-2-6-9/h3-4,7-9H,1-2,5-6H2,

InchiKey: BILOBPFKHTWHOV-UHFFFAOYSA-N

Formula: C12H14FNO

SMILES: O=C(Nc1ccccc1F)C1CCCC1

Mol. weight [g/mol]: 207.24

Physical Properties

Property code	Value	Unit	Source
gf	-44.85	kJ/mol	Joback Method
hf	-260.69	kJ/mol	Joback Method
hfus	24.20	kJ/mol	Joback Method
hvap	57.87	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.954		Crippen Method
mcvol	158.640	ml/mol	McGowan Method
pc	2944.08	kPa	Joback Method
rinpol	1629.00		NIST Webbook
rinpol	1629.00		NIST Webbook
tb	624.21	K	Joback Method
tc	852.13	K	Joback Method
tf	378.02	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.05	J/mol×K	624.21	Joback Method
cpg	432.48	J/mol×K	662.20	Joback Method
cpg	447.72	J/mol×K	700.18	Joback Method
cpg	461.84	J/mol×K	738.17	Joback Method
cpg	474.88	J/mol×K	776.15	Joback Method
cpg	486.91	J/mol×K	814.14	Joback Method
cpg	497.99	J/mol×K	852.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308607&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