Benzamide, N-(4-fluorophenyl)-2-methyl-

Inchi: InChI=1S/C14H12FNO/c1-10-4-2-3-5-13(10)14(17)16-12-8-6-11(15)7-9-12/h2-9H,1H3,(H
InchiKey: NXORULDOCYGHRM-UHFFFAOYSA-N
Formula: C14H12FNO
SMILES: Cc1ccccc1C(=O)Nc1ccc(F)cc1
Mol. weight [g/mol]: 229.25

Physical Properties

Property code	Value	Unit	Source
gf	38.22	kJ/mol	Joback Method
hf	-137.39	kJ/mol	Joback Method
hfus	29.10	kJ/mol	Joback Method
hvap	65.00	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.386		Crippen Method
mcvol	173.920	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
rinpol	1938.00		NIST Webbook
tb	686.35	K	Joback Method
tc	920.64	K	Joback Method
tf	428.60	K	Joback Method
vc	0.662	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.17	J/mol×K	686.35	Joback Method
cpg	461.07	J/mol×K	725.40	Joback Method
cpg	473.88	J/mol×K	764.45	Joback Method
cpg	485.66	J/mol×K	803.49	Joback Method
cpg	496.48	J/mol×K	842.54	Joback Method
cpg	506.39	J/mol×K	881.59	Joback Method
cpg	515.44	J/mol×K	920.64	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307002&Units=SI

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