Benzamide, 3-fluoro-N-butyl-N-methyl-

Inchi: InChI=1S/C12H16FNO/c1-3-4-8-14(2)12(15)10-6-5-7-11(13)9-10/h5-7,9H,3-4,8H2,1-2H3
InchiKey: GCAYUQJQLZZJEF-UHFFFAOYSA-N
Formula: C12H16FNO
SMILES: CCCCN(C)C(=O)c1cccc(F)c1
Mol. weight [g/mol]: 209.26

Physical Properties

Property code	Value	Unit	Source
gf	-60.01	kJ/mol	Joback Method
hf	-307.11	kJ/mol	Joback Method
hfus	28.19	kJ/mol	Joback Method
hvap	53.22	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.698		Crippen Method
mcvol	169.500	ml/mol	McGowan Method
pc	2407.64	kPa	Joback Method
rinpol	1783.00		NIST Webbook
rinpol	1783.00		NIST Webbook
tb	571.20	K	Joback Method
tc	767.95	K	Joback Method
tf	346.93	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.41	J/mol×K	571.20	Joback Method
cpg	427.45	J/mol×K	603.99	Joback Method
cpg	441.62	J/mol×K	636.78	Joback Method
cpg	454.96	J/mol×K	669.58	Joback Method
cpg	467.51	J/mol×K	702.37	Joback Method
cpg	479.30	J/mol×K	735.16	Joback Method
cpg	490.36	J/mol×K	767.95	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=U415858&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