Benzamide, 3-fluoro-N-butyl-N-isobutyl-

Inchi: InChI=1S/C15H22FNO/c1-4-5-9-17(11-12(2)3)15(18)13-7-6-8-14(16)10-13/h6-8,10,12H,
InchiKey: KQYALZYLUKUUSA-UHFFFAOYSA-N
Formula: C15H22FNO
SMILES: CCCCN(CC(C)C)C(=O)c1cccc(F)c1
Mol. weight [g/mol]: 251.34

Physical Properties

Property code	Value	Unit	Source
gf	-37.19	kJ/mol	Joback Method
hf	-374.31	kJ/mol	Joback Method
hfus	32.43	kJ/mol	Joback Method
hvap	59.51	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.724		Crippen Method
mcvol	211.770	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	1986.00		NIST Webbook
rinpol	1986.00		NIST Webbook
tb	639.40	K	Joback Method
tc	832.49	K	Joback Method
tf	365.74	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.49	J/mol×K	639.40	Joback Method
cpg	582.33	J/mol×K	671.58	Joback Method
cpg	598.21	J/mol×K	703.76	Joback Method
cpg	613.17	J/mol×K	735.95	Joback Method
cpg	627.25	J/mol×K	768.13	Joback Method
cpg	640.48	J/mol×K	800.31	Joback Method
cpg	652.92	J/mol×K	832.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415861&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

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