Benzamide, 2-fluoro-N-ethyl-N-butyl-

Inchi: InChI=1S/C13H18FNO/c1-3-5-10-15(4-2)13(16)11-8-6-7-9-12(11)14/h6-9H,3-5,10H2,1-2
InchiKey: UNLNZZIYEZBRDB-UHFFFAOYSA-N
Formula: C13H18FNO
SMILES: CCCCN(CC)C(=O)c1ccccc1F
Mol. weight [g/mol]: 223.29

Physical Properties

Property code	Value	Unit	Source
gf	-51.59	kJ/mol	Joback Method
hf	-327.75	kJ/mol	Joback Method
hfus	30.78	kJ/mol	Joback Method
hvap	55.44	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.088		Crippen Method
mcvol	183.590	ml/mol	McGowan Method
pc	2195.89	kPa	Joback Method
rinpol	1845.00		NIST Webbook
rinpol	1845.00		NIST Webbook
tb	594.08	K	Joback Method
tc	788.27	K	Joback Method
tf	358.20	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.82	J/mol×K	594.08	Joback Method
cpg	477.42	J/mol×K	626.44	Joback Method
cpg	492.14	J/mol×K	658.81	Joback Method
cpg	506.01	J/mol×K	691.17	Joback Method
cpg	519.06	J/mol×K	723.54	Joback Method
cpg	531.33	J/mol×K	755.90	Joback Method
cpg	542.87	J/mol×K	788.27	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=U415373&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