Benzamide, 2-fluoro-N-ethyl-N-isobutyl-

Inchi: InChI=1S/C13H18FNO/c1-4-15(9-10(2)3)13(16)11-7-5-6-8-12(11)14/h5-8,10H,4,9H2,1-3
InchiKey: SBWPFQOTBAVQHV-UHFFFAOYSA-N
Formula: C13H18FNO
SMILES: CCN(CC(C)C)C(=O)c1ccccc1F
Mol. weight [g/mol]: 223.29

Physical Properties

Property code	Value	Unit	Source
gf	-54.03	kJ/mol	Joback Method
hf	-333.03	kJ/mol	Joback Method
hfus	27.25	kJ/mol	Joback Method
hvap	55.05	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	2.944		Crippen Method
mcvol	183.590	ml/mol	McGowan Method
pc	2212.45	kPa	Joback Method
rinpol	1794.00		NIST Webbook
rinpol	1794.00		NIST Webbook
tb	593.64	K	Joback Method
tc	791.59	K	Joback Method
tf	343.20	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.20	J/mol×K	593.64	Joback Method
cpg	478.16	J/mol×K	626.63	Joback Method
cpg	493.19	J/mol×K	659.62	Joback Method
cpg	507.32	J/mol×K	692.62	Joback Method
cpg	520.60	J/mol×K	725.61	Joback Method
cpg	533.07	J/mol×K	758.60	Joback Method
cpg	544.76	J/mol×K	791.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415372&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