Benzamide, 3-fluoro-N-butyl-N-propyl-

Inchi: InChI=1S/C14H20FNO/c1-3-5-10-16(9-4-2)14(17)12-7-6-8-13(15)11-12/h6-8,11H,3-5,9-1
InchiKey: QLDSBBNBDRMQQG-UHFFFAOYSA-N
Formula: C14H20FNO
SMILES: CCCCN(CCC)C(=O)c1cccc(F)c1
Mol. weight [g/mol]: 237.31

Physical Properties

Property code	Value	Unit	Source
gf	-43.17	kJ/mol	Joback Method
hf	-348.39	kJ/mol	Joback Method
hfus	33.37	kJ/mol	Joback Method
hvap	57.67	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.478		Crippen Method
mcvol	197.680	ml/mol	McGowan Method
pc	2010.90	kPa	Joback Method
rinpol	2527.00		NIST Webbook
rinpol	2527.00		NIST Webbook
tb	616.96	K	Joback Method
tc	808.81	K	Joback Method
tf	369.47	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	512.73	J/mol×K	616.96	Joback Method
cpg	528.82	J/mol×K	648.94	Joback Method
cpg	544.01	J/mol×K	680.91	Joback Method
cpg	558.33	J/mol×K	712.89	Joback Method
cpg	571.82	J/mol×K	744.86	Joback Method
cpg	584.52	J/mol×K	776.84	Joback Method
cpg	596.46	J/mol×K	808.81	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=U415860&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