Benzamide, 3-fluoro-N-butyl-N-3-methylbutyl-

Inchi: InChI=1S/C16H24FNO/c1-4-5-10-18(11-9-13(2)3)16(19)14-7-6-8-15(17)12-14/h6-8,12-13
InchiKey: CKANLVJQPJWEPD-UHFFFAOYSA-N
Formula: C16H24FNO
SMILES: CCCCN(CCC(C)C)C(=O)c1cccc(F)c1
Mol. weight [g/mol]: 265.37

Physical Properties

Property code	Value	Unit	Source
gf	-28.77	kJ/mol	Joback Method
hf	-394.95	kJ/mol	Joback Method
hfus	35.02	kJ/mol	Joback Method
hvap	61.73	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.114		Crippen Method
mcvol	225.860	ml/mol	McGowan Method
pc	1716.03	kPa	Joback Method
rinpol	2234.00		NIST Webbook
rinpol	2234.00		NIST Webbook
tb	662.28	K	Joback Method
tc	853.41	K	Joback Method
tf	377.01	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.17	J/mol×K	662.28	Joback Method
cpg	636.36	J/mol×K	694.13	Joback Method
cpg	652.58	J/mol×K	725.99	Joback Method
cpg	667.86	J/mol×K	757.84	Joback Method
cpg	682.25	J/mol×K	789.70	Joback Method
cpg	695.80	J/mol×K	821.55	Joback Method
cpg	708.53	J/mol×K	853.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415863&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