Benzamide, 3-chloro-2-fluoro-N-butyl-

Inchi: InChI=1S/C11H13ClFNO/c1-2-3-7-14-11(15)8-5-4-6-9(12)10(8)13/h4-6H,2-3,7H2,1H3,(H
InchiKey: TWXUTIXZZWDHHY-UHFFFAOYSA-N
Formula: C11H13ClFNO
SMILES: CCCCNC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 229.68

Physical Properties

Property code	Value	Unit	Source
gf	-111.38	kJ/mol	Joback Method
hf	-327.74	kJ/mol	Joback Method
hfus	31.48	kJ/mol	Joback Method
hvap	60.43	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.009		Crippen Method
mcvol	167.650	ml/mol	McGowan Method
pc	2553.34	kPa	Joback Method
rinpol	1753.00		NIST Webbook
tb	628.46	K	Joback Method
tc	836.02	K	Joback Method
tf	398.29	K	Joback Method
vc	0.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.47	J/mol×K	628.46	Joback Method
cpg	416.99	J/mol×K	663.05	Joback Method
cpg	428.75	J/mol×K	697.65	Joback Method
cpg	439.78	J/mol×K	732.24	Joback Method
cpg	450.10	J/mol×K	766.83	Joback Method
cpg	459.75	J/mol×K	801.42	Joback Method
cpg	468.76	J/mol×K	836.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407821&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