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

Inchi: InChI=1S/C11H13ClFNO/c1-7(2)6-14-11(15)8-4-3-5-9(12)10(8)13/h3-5,7H,6H2,1-2H3,(H
InchiKey: KFCVWUKBTQKXQQ-UHFFFAOYSA-N
Formula: C11H13ClFNO
SMILES: CC(C)CNC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 229.68

Physical Properties

Property code	Value	Unit	Source
gf	-113.82	kJ/mol	Joback Method
hf	-333.02	kJ/mol	Joback Method
hfus	27.96	kJ/mol	Joback Method
hvap	60.04	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	2.865		Crippen Method
mcvol	167.650	ml/mol	McGowan Method
pc	2574.11	kPa	Joback Method
rinpol	1700.00		NIST Webbook
rinpol	1700.00		NIST Webbook
tb	628.02	K	Joback Method
tc	839.65	K	Joback Method
tf	383.29	K	Joback Method
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.96	J/mol×K	628.02	Joback Method
cpg	417.77	J/mol×K	663.29	Joback Method
cpg	429.77	J/mol×K	698.56	Joback Method
cpg	441.01	J/mol×K	733.84	Joback Method
cpg	451.51	J/mol×K	769.11	Joback Method
cpg	461.30	J/mol×K	804.38	Joback Method
cpg	470.40	J/mol×K	839.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407820&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

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