Benzamide, 3,4-difluoro-N-isobutyl-

Inchi: InChI=1S/C11H13F2NO/c1-7(2)6-14-11(15)8-3-4-9(12)10(13)5-8/h3-5,7H,6H2,1-2H3,(H,
InchiKey: OGPZEGWBIMALDE-UHFFFAOYSA-N
Formula: C11H13F2NO
SMILES: CC(C)CNC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 213.22

Physical Properties

Property code	Value	Unit	Source
gf	-296.70	kJ/mol	Joback Method
hf	-513.39	kJ/mol	Joback Method
hfus	26.84	kJ/mol	Joback Method
hvap	54.84	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	2.351		Crippen Method
mcvol	157.180	ml/mol	McGowan Method
pc	2553.34	kPa	Joback Method
rinpol	1572.00		NIST Webbook
tb	589.86	K	Joback Method
tc	788.30	K	Joback Method
tf	353.96	K	Joback Method
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.02	J/mol×K	589.86	Joback Method
cpg	400.09	J/mol×K	622.93	Joback Method
cpg	412.43	J/mol×K	656.01	Joback Method
cpg	424.05	J/mol×K	689.08	Joback Method
cpg	434.99	J/mol×K	722.15	Joback Method
cpg	445.26	J/mol×K	755.23	Joback Method
cpg	454.88	J/mol×K	788.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407789&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