Benzamide, 3-chloro-2-fluoro-N-(3-methylbutyl)-

Inchi: InChI=1S/C12H15ClFNO/c1-8(2)6-7-15-12(16)9-4-3-5-10(13)11(9)14/h3-5,8H,6-7H2,1-2

InchiKey: PLEBVHFELHPUEB-UHFFFAOYSA-N

Formula: C12H15ClFNO

SMILES: CC(C)CCNC(=O)c1cccc(Cl)c1F

Mol. weight [g/mol]: 243.71

Physical Properties

Property code	Value	Unit	Source
gf	-105.40	kJ/mol	Joback Method
hf	-353.66	kJ/mol	Joback Method
hfus	30.55	kJ/mol	Joback Method
hvap	62.27	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.255		Crippen Method
mcvol	181.740	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
rinpol	1817.00		NIST Webbook
rinpol	1817.00		NIST Webbook
tb	650.90	K	Joback Method
tc	859.26	K	Joback Method
tf	394.56	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.52	J/mol×K	650.90	Joback Method
cpg	467.95	J/mol×K	685.63	Joback Method
cpg	480.55	J/mol×K	720.35	Joback Method
cpg	492.35	J/mol×K	755.08	Joback Method
cpg	503.39	J/mol×K	789.81	Joback Method
cpg	513.69	J/mol×K	824.53	Joback Method
cpg	523.28	J/mol×K	859.26	Joback Method

Sources

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=U407822&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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