Benzamide, 3-methoxy-N-isobutyl-

Inchi: InChI=1S/C12H17NO2/c1-9(2)8-13-12(14)10-5-4-6-11(7-10)15-3/h4-7,9H,8H2,1-3H3,(H,
InchiKey: BNFJAAKDMOPMEN-UHFFFAOYSA-N
Formula: C12H17NO2
SMILES: COc1cccc(C(O)=NCC(C)C)c1
Mol. weight [g/mol]: 207.27

Physical Properties

Property code	Value	Unit	Source
hf	-283.25	kJ/mol	Joback Method
hvap	67.34	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	2.656		Crippen Method
mcvol	173.600	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
rinpol	1844.00		NIST Webbook
tb	696.34	K	Joback Method
tc	903.86	K	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=U407508&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation 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