Benzamide, 3,4-dimethoxy-N-isobutyl-

Inchi: InChI=1S/C13H19NO3/c1-9(2)8-14-13(15)10-5-6-11(16-3)12(7-10)17-4/h5-7,9H,8H2,1-4
InchiKey: VBWABQJMGFHEJR-UHFFFAOYSA-N
Formula: C13H19NO3
SMILES: COc1ccc(C(=O)NCC(C)C)cc1OC
Mol. weight [g/mol]: 237.29

Physical Properties

Property code	Value	Unit	Source
gf	-100.24	kJ/mol	Joback Method
hf	-426.89	kJ/mol	Joback Method
hfus	28.24	kJ/mol	Joback Method
hvap	65.75	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.090		Crippen Method
mcvol	193.560	ml/mol	McGowan Method
pc	2235.52	kPa	Joback Method
rinpol	2087.00		NIST Webbook
rinpol	2087.00		NIST Webbook
tb	681.92	K	Joback Method
tc	888.57	K	Joback Method
tf	419.78	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.03	J/mol×K	681.92	Joback Method
cpg	538.07	J/mol×K	716.36	Joback Method
cpg	552.23	J/mol×K	750.80	Joback Method
cpg	565.52	J/mol×K	785.25	Joback Method
cpg	577.94	J/mol×K	819.69	Joback Method
cpg	589.49	J/mol×K	854.13	Joback Method
cpg	600.17	J/mol×K	888.57	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=U408001&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