Benzamide, 3,4-dimethoxy-N-propyl-

Inchi: InChI=1S/C12H17NO3/c1-4-7-13-12(14)9-5-6-10(15-2)11(8-9)16-3/h5-6,8H,4,7H2,1-3H3
InchiKey: IXLDZEGNMDSKHS-UHFFFAOYSA-N
Formula: C12H17NO3
SMILES: CCCN=C(O)c1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 223.27

Physical Properties

Property code	Value	Unit	Source
hf	-421.66	kJ/mol	Joback Method
hvap	70.80	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	2.418		Crippen Method
mcvol	179.470	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	2046.00		NIST Webbook
rinpol	2046.00		NIST Webbook
tb	724.18	K	Joback Method
tc	927.60	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=U408000&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