

Benzamide, 3,4-dimethoxy-N-ethyl-

Inchi:	lnChI=1S/C11H15NO3/c1-4-12-11(13)8-5-6-9(14-2)10(7-8)15-3/h5-7H,4H2,1-3H3,(H,12,13)
InchiKey:	RZHREWGTKUEFOO-UHFFFAOYSA-N
Formula:	C11H15NO3
SMILES:	CCN=C(O)c1ccc(OC)c(OC)c1
Mol. weight [g/mol]:	209.24

Physical Properties

Property code	Value	Unit	Source
hf	-401.02	kJ/mol	Joback Method
hvap	68.57	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	2.028		Crippen Method
mcvol	165.380	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
rinpol	1951.00		NIST Webbook
tb	701.30	K	Joback Method
tc	907.05	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407999&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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