

Benzamide, 3,4-dimethoxy-N-hexyl-

Inchi:	InChI=1S/C15H23NO3/c1-4-5-6-7-10-16-15(17)12-8-9-13(18-2)14(11-12)19-3/h8-9,11H,
InchiKey:	WBTZKHUPMLWGPK-UHFFFAOYSA-N
Formula:	C15H23NO3
SMILES:	CCCCCN=C(O)c1ccc(OC)c(OC)c1
Mol. weight [g/mol]:	265.35

Physical Properties

Property code	Value	Unit	Source
hf	-483.58	kJ/mol	Joback Method
hvap	77.48	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.589		Crippen Method
mcvol	221.740	ml/mol	McGowan Method
pc	1737.56	kPa	Joback Method
rinpol	2357.00		NIST Webbook
rinpol	2357.00		NIST Webbook
tb	792.82	K	Joback Method
tc	992.22	K	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U408006&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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