

Benzamide, 3,4-dimethoxy-N-nonyl-

Inchi: InChI=1S/C18H29NO3/c1-4-5-6-7-8-9-10-13-19-18(20)15-11-12-16(21-2)17(14-15)22-3/
InchiKey: QZSAHGJHEMABDR-UHFFFAOYSA-N
Formula: C18H29NO3
SMILES: CCCCCCCCN=C(O)c1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 307.43

Physical Properties

Property code	Value	Unit	Source
hf	-545.50	kJ/mol	Joback Method
hvap	84.15	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.759		Crippen Method
mcvol	264.010	ml/mol	McGowan Method
pc	1385.05	kPa	Joback Method
rinpol	2664.00		NIST Webbook
rinpol	2664.00		NIST Webbook
tb	861.46	K	Joback Method
tc	1062.30	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U408010&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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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