

Benzamide, 3,4-dimethoxy-N-hexadecyl-

Inchi: InChI=1S/C25H43NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-26-25(27)22-18-19-2
InchiKey: YVXIITSCMUEGCF-UHFFFAOYSA-N
Formula: C25H43NO3
SMILES: CCCCCCCCCCCCCCN=C(O)c1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 405.61

Physical Properties

Property code	Value	Unit	Source
hf	-689.98	kJ/mol	Joback Method
hvap	99.74	kJ/mol	Joback Method
log10ws	-7.88		Crippen Method
logp	7.490		Crippen Method
mcvol	362.640	ml/mol	McGowan Method
pc	886.30	kPa	Joback Method
rinpol	3383.00		NIST Webbook
rinpol	3383.00		NIST Webbook
tb	1021.62	K	Joback Method
tc	1255.52	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U408015&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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