Benzamide, 3-methoxy-N-heptyl-

Inchi: InChI=1S/C15H23NO2/c1-3-4-5-6-7-11-16-15(17)13-9-8-10-14(12-13)18-2/h8-10,12H,3-
InchiKey: MIQFUGICJVSWSP-UHFFFAOYSA-N
Formula: C15H23NO2
SMILES: CCCCCCCN=C(O)c1cccc(OC)c1
Mol. weight [g/mol]: 249.35

Physical Properties

Property code	Value	Unit	Source
hf	-339.89	kJ/mol	Joback Method
hvap	74.41	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.970		Crippen Method
mcvol	215.870	ml/mol	McGowan Method
pc	1784.86	kPa	Joback Method
rinpol	2227.00		NIST Webbook
rinpol	2227.00		NIST Webbook
tb	765.42	K	Joback Method
tc	964.15	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407515&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