Benzamide, 3-methoxy-N-undecyl-

Inchi: InChI=1S/C19H31NO2/c1-3-4-5-6-7-8-9-10-11-15-20-19(21)17-13-12-14-18(16-17)22-2/h
InchiKey: QCLDFJSPCPGILJ-UHFFFAOYSA-N
Formula: C19H31NO2
SMILES: CCCCCCCCCCCN=C(O)c1cccc(OC)c1
Mol. weight [g/mol]: 305.45

Physical Properties

Property code	Value	Unit	Source
hf	-422.45	kJ/mol	Joback Method
hvap	83.31	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	5.531		Crippen Method
mcvol	272.230	ml/mol	McGowan Method
pc	1321.35	kPa	Joback Method
rinpol	2758.00		NIST Webbook
rinpol	2758.00		NIST Webbook
tb	856.94	K	Joback Method
tc	1056.57	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407519&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