

Benzamide, 3-methoxy-N-dodecyl-

Inchi: InChI=1S/C20H33NO2/c1-3-4-5-6-7-8-9-10-11-12-16-21-20(22)18-14-13-15-19(17-18)23
InchiKey: XTDIHJWVBUGDLF-UHFFFAOYSA-N
Formula: C20H33NO2
SMILES: CCCCCCCCCCN=C(O)c1cccc(OC)c1
Mol. weight [g/mol]: 319.48

Physical Properties

Property code	Value	Unit	Source
hf	-443.09	kJ/mol	Joback Method
hvap	85.53	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	5.921		Crippen Method
mcvol	286.320	ml/mol	McGowan Method
pc	1233.74	kPa	Joback Method
rinpol	2648.00		NIST Webbook
rinpol	2648.00		NIST Webbook
tb	879.82	K	Joback Method
tc	1081.43	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=U407520&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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