

Benzamide, 3-methoxy-N-(hept-2-yl)-

Inchi:	InChI=1S/C15H23NO2/c1-4-5-6-8-12(2)16-15(17)13-9-7-10-14(11-13)18-3/h7,9-12H,4-6
InchiKey:	GYSRQHDAQQUDSR-UHFFFAOYSA-N
Formula:	C15H23NO2
SMILES:	CCCCC(C)N=C(O)c1cccc(OC)c1
Mol. weight [g/mol]:	249.35

Physical Properties

Property code	Value	Unit	Source
hf	-345.17	kJ/mol	Joback Method
hvap	74.02	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.969		Crippen Method
mcvol	215.870	ml/mol	McGowan Method
pc	1796.98	kPa	Joback Method
rinpol	2084.00		NIST Webbook
rinpol	2084.00		NIST Webbook
tb	764.98	K	Joback Method
tc	966.35	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=U407512&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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