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

Inchi: InChI=1S/C15H23NO/c1-4-5-6-9-13(3)16-15(17)14-10-7-8-12(2)11-14/h7-8,10-11,13H,4-
InchiKey: XTYKMWCXIQUSNF-UHFFFAOYSA-N
Formula: C15H23NO
SMILES: CCCCCC(C)N=C(O)c1cccc(C)c1
Mol. weight [g/mol]: 233.35

Physical Properties

Property code	Value	Unit	Source
hf	-212.95	kJ/mol	Joback Method
hvap	71.61	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	4.268		Crippen Method
mcvol	210.000	ml/mol	McGowan Method
pc	1823.17	kPa	Joback Method
rinpol	1943.00		NIST Webbook
rinpol	1943.00		NIST Webbook
tb	742.56	K	Joback Method
tc	944.73	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407414&Units=SI

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