Benzamide, 3-methyl-N-heptyl-

Inchi: InChI=1S/C15H23NO/c1-3-4-5-6-7-11-16-15(17)14-10-8-9-13(2)12-14/h8-10,12H,3-7,11
InchiKey: OYABQGPEXFSLEK-UHFFFAOYSA-N
Formula: C15H23NO
SMILES: CCCCCCCN=C(O)c1cccc(C)c1
Mol. weight [g/mol]: 233.35

Physical Properties

Property code	Value	Unit	Source
hf	-207.67	kJ/mol	Joback Method
hvap	72.00	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.270		Crippen Method
mcvol	210.000	ml/mol	McGowan Method
pc	1810.77	kPa	Joback Method
rinpol	2083.00		NIST Webbook
rinpol	2083.00		NIST Webbook
tb	743.00	K	Joback Method
tc	942.28	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=U407417&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