

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

Inchi:	InChI=1S/C15H23NO/c1-4-5-6-10-13(3)16-15(17)14-11-8-7-9-12(14)2/h7-9,11,13H,4-6,1
InchiKey:	QOKZLYCJDYLZMB-UHFFFAOYSA-N
Formula:	C15H23NO
SMILES:	CCCCC(C)N=C(O)c1ccccc1C
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	1886.00		NIST Webbook
tb	742.56	K	Joback Method
tc	944.73	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=U407397&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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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