

N-Benzylbenzamide

Other names:	Benzamide, N-(phenylmethyl)- Benzamide, N-benzyl-
Inchi:	InChI=1S/C14H13NO/c16-14(13-9-5-2-6-10-13)15-11-12-7-3-1-4-8-12/h1-10H,11H2,(H,1
InchiKey:	LKQUCICFTHBFAL-UHFFFAOYSA-N
Formula:	C14H13NO
SMILES:	OC(=NCc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	211.26
CAS:	1485-70-7

Physical Properties

Property code	Value	Unit	Source
hf	60.97	kJ/mol	Joback Method
hvap	71.38	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.191		Crippen Method
mcvol	172.150	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
rinpol	2039.40		NIST Webbook
rinpol	2039.40		NIST Webbook
tb	741.82	K	Joback Method
tc	978.15	K	Joback Method

Sources

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=C1485707&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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