Benzamide, 3-methyl-N-isobutyl-

Inchi: InChI=1S/C12H17NO/c1-9(2)8-13-12(14)11-6-4-5-10(3)7-11/h4-7,9H,8H2,1-3H3,(H,13,1
InchiKey: NIHPGNMGODURLK-UHFFFAOYSA-N
Formula: C12H17NO
SMILES: Cc1cccc(C(O)=NCC(C)C)c1
Mol. weight [g/mol]: 191.27

Physical Properties

Property code	Value	Unit	Source
hf	-151.03	kJ/mol	Joback Method
hvap	64.93	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.956		Crippen Method
mcvol	167.730	ml/mol	McGowan Method
pc	2370.28	kPa	Joback Method
rinpol	1708.00		NIST Webbook
rinpol	1708.00		NIST Webbook
tb	673.92	K	Joback Method
tc	883.38	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=U407410&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Latest version available from:
https://www.chemeo.com/cid/85-459-9/Benzamide-3-methyl-N-isobutyl.pdf
Generated by Cheméo on 2024-04-25 09:12:15.617994564 +0000 UTC m=+16325584.538571879.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.