Benzamide, 3-bromo-N-pentyl-

Inchi: InChI=1S/C12H16BrNO/c1-2-3-4-8-14-12(15)10-6-5-7-11(13)9-10/h5-7,9H,2-4,8H2,1H3,
InchiKey: FPVZVKLBFHUYOM-UHFFFAOYSA-N
Formula: C12H16BrNO
SMILES: CCCCCN=C(O)c1cccc(Br)c1
Mol. weight [g/mol]: 270.17

Physical Properties

Property code	Value	Unit	Source
hf	-119.42	kJ/mol	Joback Method
hvap	71.75	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.944		Crippen Method
mcvol	185.230	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
rinpol	2057.00		NIST Webbook
rinpol	2057.00		NIST Webbook
tb	740.52	K	Joback Method
tc	956.69	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=U407206&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

Latest version available from:
https://www.chemeo.com/cid/93-964-9/Benzamide-3-bromo-N-pentyl.pdf
Generated by Cheméo on 2024-04-19 21:30:14.955583874 +0000 UTC m=+15851463.876161189.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.