

p-bromobenzylidene-propyl-amine

Inchi:	InChI=1S/C10H12BrN/c1-2-7-12-8-9-3-5-10(11)6-4-9/h3-6,8H,2,7H2,1H3/b12-8+
InchiKey:	DAKVGMUXIVYXHK-XYOKQWHBSA-N
Formula:	C10H12BrN
SMILES:	CCCN=Cc1ccc(Br)cc1
Mol. weight [g/mol]:	226.11

Physical Properties

Property code	Value	Unit	Source
hf	83.88	kJ/mol	Joback Method
hvap	50.54	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.278		Crippen Method
mcvol	151.180	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
rinpol	1572.00		NIST Webbook
tb	602.70	K	Joback Method
tc	841.76	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=R159712&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

Latest version available from:

<https://www.cheméo.com/cid/40-136-6/p-bromobenzylidene-propyl-amine.pdf>

Generated by Cheméo on 2024-04-25 18:57:04.799114123 +0000 UTC m=+16360673.719691435.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.