

p-bromobenzylidene-butyl-amine

Inchi:	InChI=1S/C11H14BrN/c1-2-3-8-13-9-10-4-6-11(12)7-5-10/h4-7,9H,2-3,8H2,1H3
InchiKey:	VJYHHNBTWPQQPS-UHFFFAOYSA-N
Formula:	C11H14BrN
SMILES:	CCCCN=Cc1ccc(Br)cc1
Mol. weight [g/mol]:	240.14

Physical Properties

Property code	Value	Unit	Source
hf	63.24	kJ/mol	Joback Method
hvap	52.77	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.668		Crippen Method
mcvol	165.270	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
rinpol	1678.00		NIST Webbook
rinpol	1678.00		NIST Webbook
tb	625.58	K	Joback Method
tc	859.73	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=R159623&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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