

p-bromobenzylidene-heptyl-amine

Inchi:	InChI=1S/C14H20BrN/c1-2-3-4-5-6-11-16-12-13-7-9-14(15)10-8-13/h7-10,12H,2-6,11H2
InchiKey:	XFQQLHLGBWQAHL-FOWTUZBSSA-N
Formula:	C14H20BrN
SMILES:	CCCCCCN=Cc1ccc(Br)cc1
Mol. weight [g/mol]:	282.22

Physical Properties

Property code	Value	Unit	Source
hf	1.32	kJ/mol	Joback Method
hvap	59.45	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.838		Crippen Method
mcvol	207.540	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
rinpol	1975.00		NIST Webbook
rinpol	1975.00		NIST Webbook
tb	694.22	K	Joback Method
tc	915.51	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=R159658&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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