

p-bromobenzylidene-nonyl-amine

Inchi: InChI=1S/C16H24BrN/c1-2-3-4-5-6-7-8-13-18-14-15-9-11-16(17)12-10-15/h9-12,14H,2-8
InchiKey: IYMXNMKNILOMKJ-NBVRZTHBSA-N
Formula: C16H24BrN
SMILES: CCCCCCCCCN=Cc1ccc(Br)cc1
Mol. weight [g/mol]: 310.27

Physical Properties

Property code	Value	Unit	Source
hf	-39.96	kJ/mol	Joback Method
hvap	63.90	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	5.619		Crippen Method
mcvol	235.720	ml/mol	McGowan Method
pc	1633.81	kPa	Joback Method
rinpol	2172.00		NIST Webbook
rinpol	2172.00		NIST Webbook
tb	739.98	K	Joback Method
tc	954.63	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R159678&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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