p-chlorobenzylidene-pentyl-amine

Inchi: InChI=1S/C12H16ClN/c1-2-3-4-9-14-10-11-5-7-12(13)8-6-11/h5-8,10H,2-4,9H2,1H3/b14-
InchiKey: QNESWJYRTZNLRY-GXDHUFHOSA-N
Formula: C12H16ClN
SMILES: CCCCCN=Cc1ccc(Cl)cc1
Mol. weight [g/mol]: 209.72

Physical Properties

Property code	Value	Unit	Source
hf	0.53	kJ/mol	Joback Method
hvap	52.94	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.949		Crippen Method
mcvol	174.100	ml/mol	McGowan Method
pc	2073.65	kPa	Joback Method
rinpol	1628.00		NIST Webbook
rinpol	1628.00		NIST Webbook
tb	619.73	K	Joback Method
tc	840.88	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R159930&Units=SI
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

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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