

p-chlorobenzylidene-(3-nitrophenyl)-amine

Inchi: InChI=1S/C13H9ClN2O2/c14-11-6-4-10(5-7-11)9-15-12-2-1-3-13(8-12)16(17)18/h1-9H/b
InchiKey: JSLHZGWGZRIVLW-OQLLNIDSSA-N
Formula: C13H9ClN2O2
SMILES: O=[N+]([O-])c1cccc(N=Cc2ccc(Cl)cc2)c1
Mol. weight [g/mol]: 260.68

Physical Properties

Property code	Value	Unit	Source
hf	194.19	kJ/mol	Joback Method
hvap	74.70	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	3.999		Crippen Method
mcvol	181.850	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
rinpol	2428.00		NIST Webbook
rinpol	2428.00		NIST Webbook
tb	826.11	K	Joback Method
tc	1108.18	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R159787&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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