3,4-Methylenedioxybenzylidene aniline

Other names: N-Piperonylideneaniline
Inchi: InChI=1S/C14H11NO2/c1-2-4-12(5-3-1)15-9-11-6-7-13-14(8-11)17-10-16-13/h1-9H,10H2
InchiKey: OCPBTGFXVLONGM-UHFFFAOYSA-N
Formula: C14H11NO2
SMILES: C(=Nc1ccccc1)c1ccc2c(c1)OCO2
Mol. weight [g/mol]: 225.24
CAS: 27738-39-2

Physical Properties

Property code	Value	Unit	Source
hf	29.19	kJ/mol	Joback Method
hvap	65.19	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.166		Crippen Method
mcvol	167.160	ml/mol	McGowan Method
pc	2799.47	kPa	Joback Method
tb	725.03	K	Joback Method
tc	990.86	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=C27738392&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature