

N-o-nitrobenzylidene-p-anisidine

Inchi: InChI=1S/C14H12N2O3/c1-19-13-8-6-12(7-9-13)15-10-11-4-2-3-5-14(11)16(17)18/h2-10
InchiKey: MOFALIQXICGDFI-XNTDXEJSSA-N
Formula: C14H12N2O3
SMILES: COc1ccc(N=Cc2ccccc2[N+](=O)[O-])cc1
Mol. weight [g/mol]: 256.26
CAS: 2501-03-3

Physical Properties

Property code	Value	Unit	Source
hf	57.07	kJ/mol	Joback Method
hvap	74.95	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.354		Crippen Method
mcvol	189.570	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
tb	833.98	K	Joback Method
tc	1103.23	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=C2501033&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

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