Benzonitrile, 4-[[(4-butoxyphenyl)methylene]amino]-

Other names: 4-[[(4-butoxybenzylidene]amino]benzonitrile
Inchi: InChI=1S/C18H18N2O/c1-2-3-12-21-18-10-6-16(7-11-18)14-20-17-8-4-15(13-19)5-9-17/h
InchiKey: JWLPZJPDDBBWQD-UHFFFAOYSA-N
Formula: C18H18N2O
SMILES: CCCCOc1ccc(C=Nc2ccc(C#N)cc2)cc1
Mol. weight [g/mol]: 278.35
CAS: 36405-17-1

Physical Properties

Property code	Value	Unit	Source
hf	150.15	kJ/mol	Joback Method
hvap	77.74	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.488		Crippen Method
mcvol	229.890	ml/mol	McGowan Method
pc	1651.11	kPa	Joback Method
tb	875.74	K	Joback Method
tc	1118.57	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C36405171&Units=SI

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