

Benzonitrile, 4-[[[4-(hexyloxy)phenyl]methylene]amino]-

Other names: 4-([4-(Hexyloxy)phenyl]methylidene)amino)benzonitrile

p-n-Hexyloxybenzylideneamino-p'-benzonitrile

4-[[4-(hexyloxy)benzylidene]amino]benzonitrile

Inchi: InChI=1S/C20H22N2O/c1-2-3-4-5-14-23-20-12-8-18(9-13-20)16-22-19-10-6-17(15-21)7-

InchiKey: YABQOLANVLHEPV-UHFFFAOYSA-N

Formula: C20H22N2O

SMILES: CCCCCCOc1ccc(C=Nc2ccc(C#N)cc2)cc1

Mol. weight [g/mol]: 306.40

CAS: 35280-78-5

Physical Properties

Property code	Value	Unit	Source
hf	108.87	kJ/mol	Joback Method
hvap	82.19	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.268		Crippen Method
mcvol	258.070	ml/mol	McGowan Method
pc	1420.78	kPa	Joback Method
ss	450.56	J/mol×K	NIST Webbook
tb	921.50	K	Joback Method
tc	1158.53	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	432.51	J/mol×K	298.15	NIST Webbook

Sources

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=C35280785&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cps:	Solid phase heat capacity
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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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