p-n-Hexyloxybenzylideneamino-p'-benzonitrile

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]:	306.41

Physical Properties

Property code	Value	Unit	Source
ie	7.91	eV	Cheméo Relay (1.0)
logp	5.268		Crippen Method
mcvol	258.070	ml/mol	McGowan Method
ss	450.56	J/mol×K	NIST Webbook
tb	697.63	K	Cheméo Relay (1.0)
tf	355.37	K	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35280785&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cps:	Solid phase heat capacity
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point