p-Octyloxybenzylidene p-cyanoaniline

Inchi: InChI=1S/C22H26N2O/c1-2-3-4-5-6-7-16-25-22-14-10-20(11-15-22)18-24-21-12-8-19(17
InchiKey: OUUJTVZTPFJGMR-UHFFFAOYSA-N
Formula: C22H26N2O
SMILES: CCCCCCCCOc1ccc(C=Nc2ccc(C#N)cc2)cc1
Mol. weight [g/mol]: 334.45
CAS: 41682-73-9

Physical Properties

Property code	Value	Unit	Source
hf	67.59	kJ/mol	Joback Method
hvap	86.64	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	6.048		Crippen Method
mcvol	286.250	ml/mol	McGowan Method
pc	1235.48	kPa	Joback Method
tb	967.26	K	Joback Method
tc	1201.51	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=C41682739&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

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