

p-n-Hexyloxybenzylideneamino-p'-fluorobenzene

Inchi:	InChI=1S/C19H22FNO/c1-2-3-4-5-14-22-19-12-6-16(7-13-19)15-21-18-10-8-17(20)9-11-
InchiKey:	LEEZEVBZFLWPH-RCCKNPSSSA-N
Formula:	C19H22FNO
SMILES:	CCCCCOC1CCC(C=Nc2ccc(F)cc2)cc1
Mol. weight [g/mol]:	299.38
CAS:	56544-26-4

Physical Properties

Property code	Value	Unit	Source
hf	-231.48	kJ/mol	Joback Method
hvap	68.67	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	5.535		Crippen Method
mcvol	244.370	ml/mol	McGowan Method
pc	1505.81	kPa	Joback Method
ss	438.76	J/mol×K	NIST Webbook
tb	795.81	K	Joback Method
tc	1016.81	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	442.55	J/mol×K	298.15	NIST Webbook
hfust	23.22	kJ/mol	328.07	NIST Webbook
sfust	70.70	J/mol×K	328.07	NIST Webbook

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:
Crippen Method:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C56544264&Units=SI>
<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

cps:	Solid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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