Benzenamine, 4-butyl-N-[(4-methoxyphenyl)methylene]-

Other names: N-(p-Methoxybenzylidene)-p-butylaniline
4-Butyl-N-[(4-methoxyphenyl)methylene]benzenamine
p-Methoxybenzylidene-p-butylaniline
p-Anisylidene-p-butylaniline
Aniline, p-butyl-N-(p-methoxybenzylidene)-
4-Methoxybenzylidene-4'-n-butylaniline
MBBA
4-Methoxybenzylidine 4'-butylaniline
4-Butyl-N-[(4-methoxyphenyl)methylidene]aniline
N-(4-Methoxybenzylidene)-p-n-butylaniline
4-Butyl-N-(p-methoxybenzylidene)aniline
DL 1047 N
N-(4-Methoxybenzylidene)-4-butylaniline
N-(4'-methoxybenzylidene)-4-butylaniline

Inchi: InChI=1S/C18H21NO/c1-3-4-5-15-6-10-17(11-7-15)19-14-16-8-12-18(20-2)13-9-16/h6-14

InchiKey: FEIWNULTQYHCDN-UHFFFAOYSA-N

Formula: C18H21NO

SMILES: CCCCc1ccc(N=Cc2ccc(OC)cc2)cc1

Mol. weight [g/mol]: 267.37

CAS: 26227-73-6

Physical Properties

Property code	Value	Unit	Source
hf	-14.73	kJ/mol	Joback Method
hvap	67.26	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	4.788		Crippen Method
mcvol	228.510	ml/mol	McGowan Method
pc	1685.18	kPa	Joback Method
tb	773.66	K	Joback Method
tc	1006.61	K	Joback Method
tt	295.30 ± 0.10	K	NIST Webbook
tt	294.00 ± 0.10	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	477.00	J/mol×K	298.15	NIST Webbook
cpl	490.00	J/mol×K	300.00	NIST Webbook
cpl	475.30	J/mol×K	298.15	NIST Webbook
hfust	18.03	kJ/mol	295.30	NIST Webbook
sfust	61.04	J/mol×K	295.30	NIST Webbook

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=C26227736&Units=SI

Legend

cpl:	Liquid 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tt:	Triple Point Temperature

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