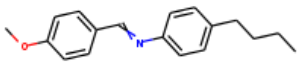
N-(4-Methoxybenzylidene)-p-n-butylaniline



Other names: 4-Butyl-N-(p-methoxybenzylidene)aniline; 4-Butyl-N-[(4-methoxyphenyl)methylene]benzenamine; 4-Butyl-N-[(4-methoxyphenyl)methylidene]aniline; 4-Methoxybenzylidene-4'-n-butylaniline; 4-Methoxybenzylidine 4'-butylaniline; Aniline, p-butyl-N-(p-methoxybenzylidene)-; DL 1047 N; MBBA; N-(4'-methoxybenzylidene)-4-butylaniline; N-(4-Methoxybenzylidene)-4-butylaniline; N-(4-Methoxybenzylidene)-p-n-butylaniline; N-(p-Methoxybenzylidene)-p-butylaniline; p-Anisylidene-p-butylaniline; p-Methoxybenzylidene-p-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/h6-14H,3-5H2,1-2H3

InChI Key: FEIWNULTQYHCDN-UHFFFAOYSA-N

Formula: C18H21NO

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

Molecular Weight: 267.37

CAS: 26227-73-6

Physical Properties

Property	Value	Unit	Source
$\Delta_f H°_{gas}$	-14.73	kJ/mol	Joback Method
$\Delta_{vap} H°$	67.26	kJ/mol	Joback Method
$logP_{oct/wat}$	4.788		Crippen Method
P_c	1685.18	kPa	Joback Method
T_{boil}	773.66	K	Joback Method
T_c	1006.61	K	Joback Method
T_{triple}	295.30 ± 0.10	K	NIST Webbook
T_{triple}	294.00 ± 0.10	K	NIST Webbook

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,liquid}$	477.00	J/mol×K	298.15	NIST Webbook
$C_{p,liquid}$	475.30	J/mol×K	298.15	NIST Webbook

Property	Value	Unit	Temperature (K)	Source
$C_{p,liquid}$	490.00	J/mol×K	300.0	NIST Webbook
$\Delta_{fus}H$	18.03	kJ/mol	295.3	NIST Webbook
$\Delta_{fus}S$	61.04	J/mol×K	295.3	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/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/h6-14H,3-5H2,1-2H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$C_{p,liquid}$: Liquid phase heat capacity (J/mol×K).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}H$: Enthalpy of fusion at a given temperature (kJ/mol).
$\Delta_{vap}H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
***log*$P_{oct/wat}$**: Octanol/Water partition coefficient .
P_c: Critical Pressure (kPa).
$\Delta_{fus}S$: Entropy of fusion at a given temperature (J/mol×K).
T_{boil}: Normal Boiling Point Temperature (K).
T_c: Critical Temperature (K).
T_{triple}: Triple Point Temperature (K).