1-CHLOROBENZENE,-4-BENZYLIDENAMINO

Other names: 1-Chlorobenzene, 4-benzylidenamino-
Benzylidene-(4-chlorophenyl)-amine
Inchi: InChI=1S/C13H10ClN/c14-12-6-8-13(9-7-12)15-10-11-4-2-1-3-5-11/h1-10H
InchiKey: NWCAQYVAHZWHIO-UHFFFAOYSA-N
Formula: C13H10ClN
SMILES: Clc1ccc(N=Cc2ccccc2)cc1
Mol. weight [g/mol]: 215.68

Physical Properties

Property code	Value	Unit	Source
af	0.4824		Cheméo Relay (1.0)
gf	305.63	kJ/mol	Cheméo Relay (1.0, beta)
hf	243.83	kJ/mol	Cheméo Relay (1.0)
hvap	77.61	kJ/mol	Cheméo Relay (1.0)
ie	8.07	eV	Cheméo Relay (1.0)
log10ws	-4.11		Cheméo Relay (1.0)
logp	4.091		Crippen Method
mcvol	164.430	ml/mol	McGowan Method
pc	2600.43	kPa	Joback Method
rinpol	1977.00		NIST Webbook
rinpol	1977.00		NIST Webbook
tb	602.96	K	Cheméo Relay (1.0)
tc	858.29	K	Cheméo Relay (1.0)
tf	345.99	K	Cheméo Relay (1.0)
vc	0.589	m3/kmol	Cheméo Relay (1.0)

Sources

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=C780212&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume