

(CH₃)₂N-CH=N-(4-bromophenyl)

Inchi: InChI=1S/C9H11BrN2/c1-12(2)7-11-9-5-3-8(10)4-6-9/h3-7H,1-2H3
InchiKey: OJKJZQJONGTMRZ-UHFFFAOYSA-N
Formula: C₉H₁₁BrN₂
SMILES: CN(C)C=Nc1ccc(Br)cc1
Mol. weight [g/mol]: 227.10
CAS: 119044-60-9

Physical Properties

Property code	Value	Unit	Source
affp	981.30	kJ/mol	NIST Webbook
basg	948.90	kJ/mol	NIST Webbook
hf	172.05	kJ/mol	Joback Method
hvap	50.36	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.671		Crippen Method
mcvol	147.070	ml/mol	McGowan Method
pc	3072.75	kPa	Joback Method
tb	592.26	K	Joback Method
tc	832.25	K	Joback Method

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: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C119044609&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

affp: Proton affinity

basg:	Gas basicity
hf:	Enthalpy of formation at standard conditions
hvac:	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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