

N,N,2,6-Tetramethylaniline,4-bromo-

Inchi:	InChI=1S/C10H14BrN/c1-7-5-9(11)6-8(2)10(7)12(3)4/h5-6H,1-4H3
InchiKey:	NDDKEDQKCHIHMI-UHFFFAOYSA-N
Formula:	C10H14BrN
SMILES:	Cc1cc(Br)cc(C)c1N(C)C
Mol. weight [g/mol]:	228.13
CAS:	50638-54-5

Physical Properties

Property code	Value	Unit	Source
affp	935.40	kJ/mol	NIST Webbook
basg	902.90	kJ/mol	NIST Webbook
gf	241.94	kJ/mol	Joback Method
hf	46.25	kJ/mol	Joback Method
hfus	22.84	kJ/mol	Joback Method
hvap	50.59	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.132		Crippen Method
mcvol	155.480	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
tb	548.42	K	Joback Method
tc	769.25	K	Joback Method
tf	358.71	K	Joback Method
vc	0.568	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.92	J/molxK	548.42	Joback Method
cpg	345.84	J/molxK	585.22	Joback Method
cpg	358.94	J/molxK	622.03	Joback Method
cpg	371.25	J/molxK	658.83	Joback Method
cpg	382.80	J/molxK	695.64	Joback Method
cpg	393.65	J/molxK	732.44	Joback Method
cpg	403.82	J/molxK	769.25	Joback Method

Sources

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=C50638545&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/94-267-2/N-N-2-6-Tetramethylaniline-4-bromo.pdf>

Generated by Cheméo on 2024-04-19 16:52:09.094711779 +0000 UTC m=+15834778.015289091.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.