3-BROMO-4-METHYLANILINE

Other names:	p-Toluidine, 3-bromo-
	3-Bromo-p-toluidine
	3-Bromo-4-methylaniline
	3-Bromo-1,4-toluidine
	3-Bromo-4-methyl-phenylamine
Inchi:	InChI=1S/C7H8BrN/c1-5-2-3-6(9)4-7(5)8/h2-4H,9H2,1H3
InchiKey:	GRXMMIBZRMKADT-UHFFFAOYSA-N
Formula:	C7H8BrN
SMILES:	Cc1ccc(N)cc1Br
Mol. weight [g/mol]:	186.05

Physical Properties

Property code	Value	Unit	Source
hf	87.86	kJ/mol	Cheméo Relay (1.0)
hfus	17.63	kJ/mol	Joback Method
ie	7.82	eV	Cheméo Relay (1.0)
log10ws	-2.42		Cheméo Relay (1.0)
logp	2.340		Crippen Method
mcvol	113.210	ml/mol	McGowan Method
tb	536.94	K	Cheméo Relay (1.0)
tf	322.67	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.00	J/mol×K	534.89	Joback Method
cpg	230.14	J/mol×K	575.92	Joback Method
cpg	239.59	J/mol×K	616.95	Joback Method
cpg	248.36	J/mol×K	657.98	Joback Method
cpg	256.52	J/mol×K	699.01	Joback Method
cpg	264.09	J/mol×K	740.04	Joback Method
cpg	271.11	J/mol×K	781.07	Joback Method

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=C7745917&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

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point