

4-BROMO-2,6-DIMETHYLANILINE

Other names:	4-Bromo-2,6-dimethylaniline 4-Bromo-2,6-xylydine 2,6-Dimethyl-4-bromoaniline 2,6-Xylydine, 4-bromo-
Inchi:	InChI=1S/C8H10BrN/c1-5-3-7(9)4-6(2)8(5)10/h3-4H,10H2,1-2H3
InchiKey:	QGLAYJCJLHNIGJ-UHFFFAOYSA-N
Formula:	C8H10BrN
SMILES:	Cc1cc(Br)cc(C)c1N
Mol. weight [g/mol]:	200.08

Physical Properties

Property code	Value	Unit	Source
af	0.4965		Cheméo Relay (1.0)
hf	60.70	kJ/mol	Cheméo Relay (1.0)
hfus	19.83	kJ/mol	Joback Method
hvap	69.32	kJ/mol	Cheméo Relay (1.0)
ie	7.76	eV	Cheméo Relay (1.0)
log10ws	-2.87		Cheméo Relay (1.0)
logp	2.648		Crippen Method
mcvol	127.300	ml/mol	McGowan Method
pc	4036.37	kPa	Joback Method
tb	532.44	K	Cheméo Relay (1.0)
tc	769.21	K	Cheméo Relay (1.0)
tf	341.70	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.03	J/mol×K	562.75	Joback Method
cpg	273.04	J/mol×K	603.12	Joback Method
cpg	283.35	J/mol×K	643.49	Joback Method
cpg	293.01	J/mol×K	683.86	Joback Method
cpg	302.04	J/mol×K	724.23	Joback Method
cpg	310.48	J/mol×K	764.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24596198&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
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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