

Aniline, 4-bromo-n-tert-butyl-

Inchi:	InChI=1S/C10H14BrN/c1-10(2,3)12-9-6-4-8(11)5-7-9/h4-7,12H,1-3H3
InchiKey:	XJQHZAQOPUDOL-UHFFFAOYSA-N
Formula:	C10H14BrN
SMILES:	CC(C)(C)Nc1ccc(Br)cc1
Mol. weight [g/mol]:	228.13
CAS:	36171-07-0

Physical Properties

Property code	Value	Unit	Source
gf	242.65	kJ/mol	Joback Method
hf	46.38	kJ/mol	Joback Method
hfus	18.28	kJ/mol	Joback Method
hvap	52.37	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.660		Crippen Method
mcvol	155.480	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
tb	572.96	K	Joback Method
tc	808.85	K	Joback Method
tf	356.28	K	Joback Method
vc	0.574	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.05	J/mol×K	572.96	Joback Method
cpg	363.71	J/mol×K	612.27	Joback Method
cpg	377.24	J/mol×K	651.59	Joback Method
cpg	389.73	J/mol×K	690.90	Joback Method
cpg	401.27	J/mol×K	730.22	Joback Method
cpg	411.93	J/mol×K	769.53	Joback Method
cpg	421.79	J/mol×K	808.85	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=C36171070&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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