

Aniline, 2-tert-butyl-4-chloro-

Inchi:	InChI=1S/C10H14ClN/c1-10(2,3)8-6-7(11)4-5-9(8)12/h4-6H,12H2,1-3H3
InchiKey:	STWRRIVJDPYRLH-UHFFFAOYSA-N
Formula:	C10H14ClN
SMILES:	CC(C)(C)c1cc(Cl)ccc1N
Mol. weight [g/mol]:	183.68

Physical Properties

Property code	Value	Unit	Source
gf	183.83	kJ/mol	Joback Method
hf	-26.84	kJ/mol	Joback Method
hfus	16.90	kJ/mol	Joback Method
hvap	55.18	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	3.220		Crippen Method
mvol	150.220	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
tb	571.57	K	Joback Method
tc	808.32	K	Joback Method
tf	369.52	K	Joback Method
vc	0.554	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.10	J/mol×K	571.57	Joback Method
cpg	360.40	J/mol×K	611.03	Joback Method
cpg	373.67	J/mol×K	650.49	Joback Method
cpg	385.97	J/mol×K	689.94	Joback Method
cpg	397.36	J/mol×K	729.40	Joback Method
cpg	407.92	J/mol×K	768.86	Joback Method
cpg	417.70	J/mol×K	808.32	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=B6008509&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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