

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

Inchi:	InChI=1S/C14H23N/c1-13(2,3)11-7-9-12(10-8-11)15-14(4,5)6/h7-10,15H,1-6H3
InchiKey:	YKQQYQHMSGJYTG-UHFFFAOYSA-N
Formula:	C14H23N
SMILES:	CC(C)(C)Nc1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]:	205.34
CAS:	36209-85-5

Physical Properties

Property code	Value	Unit	Source
gf	264.85	kJ/mol	Joback Method
hf	-71.26	kJ/mol	Joback Method
hfus	15.94	kJ/mol	Joback Method
hvap	53.54	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	4.194		Crippen Method
mcvol	194.340	ml/mol	McGowan Method
pc	2075.54	kPa	Joback Method
tb	595.09	K	Joback Method
tc	814.52	K	Joback Method
tf	343.98	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.83	J/molxK	595.09	Joback Method
cpg	524.26	J/molxK	631.66	Joback Method
cpg	542.34	J/molxK	668.23	Joback Method
cpg	559.16	J/molxK	704.80	Joback Method
cpg	574.80	J/molxK	741.37	Joback Method
cpg	589.37	J/molxK	777.95	Joback Method
cpg	602.94	J/molxK	814.52	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=C36209855&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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