

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

Inchi:	InChI=1S/C10H14ClN/c1-10(2,3)12-9-6-4-8(11)5-7-9/h4-7,12H,1-3H3
InchiKey:	BWQVJYBZWVXQPE-UHFFFAOYSA-N
Formula:	C10H14ClN
SMILES:	CC(C)(C)Nc1ccc(Cl)cc1
Mol. weight [g/mol]:	183.68
CAS:	48131-06-2

Physical Properties

Property code	Value	Unit	Source
gf	216.40	kJ/mol	Joback Method
hf	4.31	kJ/mol	Joback Method
hfus	17.19	kJ/mol	Joback Method
hvap	50.32	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.550		Crippen Method
mvol	150.220	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
tb	544.23	K	Joback Method
tc	770.30	K	Joback Method
tf	326.40	K	Joback Method
vc	0.560	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.26	J/mol×K	544.23	Joback Method
cpg	351.24	J/mol×K	581.91	Joback Method
cpg	365.16	J/mol×K	619.59	Joback Method
cpg	378.07	J/mol×K	657.27	Joback Method
cpg	390.05	J/mol×K	694.94	Joback Method
cpg	401.14	J/mol×K	732.62	Joback Method
cpg	411.43	J/mol×K	770.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C48131062&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/85-756-9/Aniline-n-tert-butyl-4-chloro.pdf>

Generated by Cheméo on 2024-04-20 04:19:24.39076371 +0000 UTC m=+15876013.311341026.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.