4-tert-Butyl-2-chlorophenol

Other names:	Phenol, 2-chloro-4-(1,1-dimethylethyl)-
	Phenol, 4-tert-butyl-2-chloro-
	2-Chloro-4-tert-butylphenol
	Phenol, 2-chloro, 4-t-butyl
Inchi:	InChI=1S/C10H13ClO/c1-10(2,3)7-4-5-9(12)8(11)6-7/h4-6,12H,1-3H3
InchiKey:	PRLINSMUYJWPBL-UHFFFAOYSA-N
Formula:	C10H13ClO
SMILES:	CC(C)(C)c1ccc(O)c(Cl)c1
Mol. weight [g/mol]:	184.66
CAS:	98-28-2

Physical Properties

Property code	Value	Unit	Source
gf	-27.61	kJ/mol	Joback Method
hf	-226.47	kJ/mol	Joback Method
hfus	17.87	kJ/mol	Joback Method
hvap	56.89	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	3.343		Crippen Method
mcvol	146.110	ml/mol	McGowan Method
pc	3337.38	kPa	Joback Method
rinpol	1487.00		NIST Webbook
rinpol	1487.00		NIST Webbook
tb	574.68	K	Joback Method
tc	812.94	K	Joback Method
tf	385.46	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.45	J/mol×K	574.68	Joback Method
cpg	353.77	J/mol×K	614.39	Joback Method
cpg	366.02	J/mol×K	654.10	Joback Method

cpg	377.32	J/mol×K	693.81	Joback Method
cpg	387.80	J/mol×K	733.52	Joback Method
cpg	397.57	J/mol×K	773.23	Joback Method
cpg	406.76	J/mol×K	812.94	Joback Method
dvisc	0.0014414	Pa×s	385.46	Joback Method
dvisc	0.0006374	Pa×s	417.00	Joback Method
dvisc	0.0003161	Pa×s	448.53	Joback Method
dvisc	0.0001719	Pa×s	480.07	Joback Method
dvisc	0.0001008	Pa×s	511.61	Joback Method
dvisc	0.0000629	Pa×s	543.14	Joback Method
dvisc	0.0000413	Pa×s	574.68	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=C98282&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
dvisc:	Dynamic viscosity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume