1-Chloro-4-(1,1-dimethylethyl)benzene

Other names:	Benzene, 1-chloro-4-(1,1-dimethylethyl)-
	Benzene, 1-tert-butyl-4-chloro-
	p-Chloro-tert-butylbenzene
	1-tert-Butyl-4-chlorobenzene
	p-tert-Butylchlorobenzene
	4-Chloro-tert-butylbenzene
	4-tert-Butyl-chlorobenzene
	4-tert-butyl-1-chlorobenzene
Inchi:	InChI=1S/C10H13Cl/c1-10(2,3)8-4-6-9(11)7-5-8/h4-7H,1-3H3
InchiKey:	XRTANKYQJQXSFP-UHFFFAOYSA-N
Formula:	C10H13Cl
SMILES:	CC(C)(C)c1ccc(Cl)cc1
Mol. weight [g/mol]:	168.66
CAS:	3972-56-3

Physical Properties

Property code	Value	Unit	Source
gf	127.01	kJ/mol	Joback Method
hf	-49.16	kJ/mol	Joback Method
hfl	-108.00 ± 3.00	kJ/mol	NIST Webbook
hfus	12.09	kJ/mol	Joback Method
hvap	43.88	kJ/mol	Joback Method
ie	8.48	eV	NIST Webbook
ie	8.56 ± 0.02	eV	NIST Webbook
ie	8.82	eV	NIST Webbook
ie	8.70	eV	NIST Webbook
log10ws	-3.47		Crippen Method
logp	3.637		Crippen Method
mcvol	140.240	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
tb	484.20	K	NIST Webbook
tb	485.00 ± 5.00	K	NIST Webbook
tb	488.00 ± 3.00	K	NIST Webbook
tc	720.15	K	Joback Method
tf	273.74	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.69	J/mol×K	494.06	Joback Method
cpg	354.69	J/mol×K	682.47	Joback Method
cpg	343.37	J/mol×K	644.79	Joback Method
cpg	331.18	J/mol×K	607.10	Joback Method
cpg	318.04	J/mol×K	569.42	Joback Method
cpg	303.90	J/mol×K	531.74	Joback Method
cpg	365.18	J/mol×K	720.15	Joback Method
dvisc	0.0002270	Pa×s	494.06	Joback Method
dvisc	0.0002967	Pa×s	457.34	Joback Method
dvisc	0.0004062	Pa×s	420.62	Joback Method
dvisc	0.0005906	Pa×s	383.90	Joback Method
dvisc	0.0009295	Pa×s	347.18	Joback Method
dvisc	0.0016285	Pa×s	310.46	Joback Method
dvisc	0.0033165	Pa×s	273.74	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=C3972563&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
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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