1-Chloro-4-tert-butoxybenzene

Inchi: InChI=1S/C10H13ClO/c1-10(2,3)12-9-6-4-8(11)5-7-9/h4-7H,1-3H3
InchiKey: NEJWTQIEQDHWTR-UHFFFAOYSA-N
Formula: C10H13ClO
SMILES: CC(C)(C)Oc1ccc(Cl)cc1
Mol. weight [g/mol]: 184.66
CAS: 18995-35-2

Physical Properties

Property code	Value	Unit	Source
gf	22.01	kJ/mol	Joback Method
hf	-181.38	kJ/mol	Joback Method
hfus	13.28	kJ/mol	Joback Method
hvap	46.29	kJ/mol	Joback Method
ie	8.72	eV	NIST Webbook
log10ws	-3.64		Crippen Method
logp	3.517		Crippen Method
mcvol	146.110	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
tb	516.48	K	Joback Method
tc	740.03	K	Joback Method
tf	295.97	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.79	J/mol×K	516.48	Joback Method
cpg	327.51	J/mol×K	553.74	Joback Method
cpg	341.29	J/mol×K	591.00	Joback Method
cpg	354.15	J/mol×K	628.25	Joback Method
cpg	366.15	J/mol×K	665.51	Joback Method
cpg	377.32	J/mol×K	702.77	Joback Method
cpg	387.72	J/mol×K	740.03	Joback Method
dvisc	0.0023736	Pa×s	295.97	Joback Method

dvisc	0.0012269	Pa×s	332.72	Joback Method
dvisc	0.0007232	Pa×s	369.47	Joback Method
dvisc	0.0004690	Pa×s	406.23	Joback Method
dvisc	0.0003269	Pa×s	442.98	Joback Method
dvisc	0.0002408	Pa×s	479.73	Joback Method
dvisc	0.0001852	Pa×s	516.48	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C18995352&Units=SI

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
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