Benzene, 1-(chloromethyl)-4-(1,1-dimethylethyl)-

Other names: p-tert-Butyl-«alpha»-chlorotoluene
p-tert-Butylbenzyl chloride
4-(tert-Butyl)benzyl chloride
Benzene,1-(chloromethyl)-4-dimethylethyl)-
p-(tert-butyl)-alpha-chlorotoluene

Inchi: InChI=1S/C11H15Cl/c1-11(2,3)10-6-4-9(8-12)5-7-10/h4-7H,8H2,1-3H3

InchiKey: WAXIFMGAKWIFDQ-UHFFFAOYSA-N

Formula: C11H15Cl

SMILES: CC(C)(C)c1ccc(CCl)cc1

Mol. weight [g/mol]: 182.69

CAS: 19692-45-6

Physical Properties

Property code	Value	Unit	Source
gf	135.43	kJ/mol	Joback Method
hf	-69.80	kJ/mol	Joback Method
hfus	14.68	kJ/mol	Joback Method
hvap	46.11	kJ/mol	Joback Method
ie	8.60 ± 0.03	eV	NIST Webbook
log10ws	-3.82		Crippen Method
logp	3.723		Crippen Method
mcvol	154.330	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
rinpol	1326.00		NIST Webbook
tb	516.94	K	Joback Method
tc	739.16	K	Joback Method
tf	285.01	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.36	J/mol×K	516.94	Joback Method
cpg	349.41	J/mol×K	553.98	Joback Method

cpg	364.38	J/mol×K	591.01	Joback Method
cpg	378.31	J/mol×K	628.05	Joback Method
cpg	391.28	J/mol×K	665.09	Joback Method
cpg	403.35	J/mol×K	702.12	Joback Method
cpg	414.58	J/mol×K	739.16	Joback Method
dvisc	0.0032297	Pa×s	285.01	Joback Method
dvisc	0.0015576	Pa×s	323.67	Joback Method
dvisc	0.0008777	Pa×s	362.32	Joback Method
dvisc	0.0005524	Pa×s	400.98	Joback Method
dvisc	0.0003772	Pa×s	439.63	Joback Method
dvisc	0.0002739	Pa×s	478.29	Joback Method
dvisc	0.0002087	Pa×s	516.94	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.20	K	0.90	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19692456&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume