Benzene, 3-chloro-1-methyl-4-(1,1-dimethylethyl)

Inchi: InChI=1S/C11H15Cl/c1-8-5-6-9(10(12)7-8)11(2,3)4/h5-7H,1-4H3
InchiKey: XQVQFDUMCCPINW-UHFFFAOYSA-N
Formula: C11H15Cl
SMILES: Cc1ccc(C(C)(C)C)c(Cl)c1
Mol. weight [g/mol]: 182.69

Physical Properties

Property code	Value	Unit	Source
gf	125.80	kJ/mol	Joback Method
hf	-81.27	kJ/mol	Joback Method
hfus	14.29	kJ/mol	Joback Method
hvap	46.77	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.946		Crippen Method
mcvol	154.330	ml/mol	McGowan Method
pc	2522.65	kPa	Joback Method
rinpol	1260.00		NIST Webbook
rinpol	1260.00		NIST Webbook
tb	521.92	K	Joback Method
tc	745.33	K	Joback Method
tf	297.53	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.56	J/mol×K	521.92	Joback Method
cpg	349.22	J/mol×K	559.16	Joback Method
cpg	363.85	J/mol×K	596.39	Joback Method
cpg	377.52	J/mol×K	633.63	Joback Method
cpg	390.27	J/mol×K	670.86	Joback Method
cpg	402.17	J/mol×K	708.10	Joback Method
cpg	413.27	J/mol×K	745.33	Joback Method
dvisc	0.0023098	Pa×s	297.53	Joback Method

dvisc	0.0012255	Pa×s	334.93	Joback Method
dvisc	0.0007385	Pa×s	372.33	Joback Method
dvisc	0.0004881	Pa×s	409.72	Joback Method
dvisc	0.0003457	Pa×s	447.12	Joback Method
dvisc	0.0002583	Pa×s	484.52	Joback Method
dvisc	0.0002012	Pa×s	521.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R132108&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
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