

Benzene, 2-chloro-1-methyl-4-(1,1-dimethylethyl)

Inchi:	InChI=1S/C11H15Cl/c1-8-5-6-9(7-10(8)12)11(2,3)4/h5-7H,1-4H3
InchiKey:	GPHQXTFRTJKHPI-UHFFFAOYSA-N
Formula:	C11H15Cl
SMILES:	Cc1ccc(C(C)(C)C)cc1Cl
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
mvol	154.330	ml/mol	McGowan Method
pc	2522.65	kPa	Joback Method
rinpol	1262.00		NIST Webbook
rinpol	1262.00		NIST Webbook
tb	521.92	K	Joback Method
tc	745.33	K	Joback Method
tf	297.53	K	Joback Method
vc	0.582	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0012255	Paxs	334.93	Joback Method
dvisc	0.0007385	Paxs	372.33	Joback Method
dvisc	0.0004881	Paxs	409.72	Joback Method
dvisc	0.0003457	Paxs	447.12	Joback Method
dvisc	0.0002583	Paxs	484.52	Joback Method
dvisc	0.0002012	Paxs	521.92	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R131972&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
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

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