Benzene, 1-chloro-2-(1-methylethyl)-

Other names:	Cumene, o-chloro-
	o-Chlorocumene
	2-Chloroisopropylbenzene
	2-chlorocumene
Inchi:	InChI=1S/C9H11Cl/c1-7(2)8-5-3-4-6-9(8)10/h3-7H,1-2H3
InchiKey:	RNEMUWDQJSRDMQ-UHFFFAOYSA-N
Formula:	C9H11Cl
SMILES:	CC(C)c1ccccc1Cl
Mol. weight [g/mol]:	154.64
CAS:	2077-13-6

Physical Properties

Property code	Value	Unit	Source
gf	113.31	kJ/mol	Joback Method
hf	-25.05	kJ/mol	Joback Method
hfl	-79.40 ± 2.10	kJ/mol	NIST Webbook
hfl	-74.80 ± 1.90	kJ/mol	NIST Webbook
hfl	-74.80 ± 1.90	kJ/mol	NIST Webbook
hfus	13.39	kJ/mol	Joback Method
hvap	42.56	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.463		Crippen Method
mcvol	126.150	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
rinpol	1102.00		NIST Webbook
rinpol	1102.00		NIST Webbook
tb	464.15 ± 2.00	K	NIST Webbook
tb	464.30	K	NIST Webbook
tc	694.11	K	Joback Method
tf	245.05	K	Joback Method
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.10	J/mol×K	657.42	Joback Method
cpg	291.74	J/mol×K	620.73	Joback Method
cpg	280.70	J/mol×K	584.04	Joback Method
cpg	268.93	J/mol×K	547.35	Joback Method
cpg	256.40	J/mol×K	510.66	Joback Method
cpg	243.09	J/mol×K	473.97	Joback Method
cpg	311.78	J/mol×K	694.11	Joback Method
dvisc	0.0033321	Pa×s	245.05	Joback Method
dvisc	0.0002333	Pa×s	473.97	Joback Method
dvisc	0.0002993	Pa×s	435.82	Joback Method
dvisc	0.0004028	Pa×s	397.66	Joback Method
dvisc	0.0005773	Pa×s	359.51	Joback Method
dvisc	0.0009014	Pa×s	321.36	Joback Method
dvisc	0.0015870	Pa×s	283.20	Joback Method
hvapt	48.10	kJ/mol	403.00	NIST Webbook
hvapt	47.70	kJ/mol	435.50	NIST Webbook

Sources

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=C2077136&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvapt: Enthalpy of vaporization at a given temperature
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