Benzene, 1-chloro-4-(1-methylethyl)-

Other names:	1-Chloro-4-isopropylbenzene
	2-(p-Chlorophenyl)propane
	4-Chloroisopropylbenzene
	4-chlorocumene
	Cumene, p-chloro-
	p-Chlorocumene
Inchi:	InChI=1S/C9H11Cl/c1-7(2)8-3-5-9(10)6-4-8/h3-7H,1-2H3
InchiKey:	FHBSIIZALGOVLM-UHFFFAOYSA-N
Formula:	C9H11Cl
SMILES:	CC(C)c1ccc(Cl)cc1
Mol. weight [g/mol]:	154.64
CAS:	2621-46-7

Physical Properties

Property code	Value	Unit	Source
gf	113.31	kJ/mol	Joback Method
hf	-25.05	kJ/mol	Joback Method
hfl	-77.90 ± 1.80	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	1080.00		NIST Webbook
tb	463.00 ± 4.00	K	NIST Webbook
tb	466.00 ± 4.00	K	NIST Webbook
tb	471.50	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	51.40	kJ/mol	389.50	NIST Webbook
hvapt	48.50	kJ/mol	440.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41947e+01
Coeff. B	-3.82371e+03
Coeff. C	-7.22130e+01
Temperature range (K), min.	347.16
Temperature range (K), max.	502.66

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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=C2621467&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
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume