Benzene, 4-(chloromethyl)-1,2-dimethyl-

Other names:	1,2-Dimethyl-4-(chloromethyl)benzene
	3,4-Dimethylbenzyl chloride
	4-(chloromethyl)-o-xylene
	Benzene, 1-(chloromethyl)-3,4-dimethyl-
Inchi:	InChI=1S/C9H11Cl/c1-7-3-4-9(6-10)5-8(7)2/h3-5H,6H2,1-2H3
InchiKey:	UBQRAAXAHIKWRI-UHFFFAOYSA-N
Formula:	C9H11Cl
SMILES:	Cc1ccc(CCl)cc1C
Mol. weight [g/mol]:	154.64
CAS:	102-46-5

Physical Properties

Property code	Value	Unit	Source
gf	106.12	kJ/mol	Joback Method
hf	-31.24	kJ/mol	Joback Method
hfus	16.53	kJ/mol	Joback Method
hvap	43.61	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.042		Crippen Method
mcvol	126.150	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
rinpol	1233.00		NIST Webbook
rinpol	1200.00		NIST Webbook
tb	479.39	K	Joback Method
tc	695.70	K	Joback Method
tf	272.57	K	Joback Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.19	J/mol×K	479.39	Joback Method
cpg	299.10	J/mol×K	659.65	Joback Method
cpg	289.18	J/mol×K	623.60	Joback Method

cpg	278.64	J/mol×K	587.55	Joback Method
cpg	267.48	J/mol×K	551.49	Joback Method
cpg	255.67	J/mol×K	515.44	Joback Method
cpg	308.45	J/mol×K	695.70	Joback Method
dvisc	0.0002356	Pa×s	479.39	Joback Method
dvisc	0.0002888	Pa×s	444.92	Joback Method
dvisc	0.0003664	Pa×s	410.45	Joback Method
dvisc	0.0004855	Pa×s	375.98	Joback Method
dvisc	0.0006809	Pa×s	341.51	Joback Method
dvisc	0.0010303	Pa×s	307.04	Joback Method
dvisc	0.0017313	Pa×s	272.57	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	389.70	K	3.20	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38272e+01
Coeff. B	-3.79701e+03
Coeff. C	-7.51370e+01
Temperature range (K), min.	355.57
Temperature range (K), max.	521.02

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C102465&Units=SI

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

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
pvap:	Vapor 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