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

Other names:	1,2-Dichloro-4-(chloromethyl)benzene
	3,4-Dichlorobenzyl chloride
	Benzene, 3,4-dichloro-1-chloromethyl
	Toluene, «alpha»,3,4-trichloro-
	Toluene, Â«alphaÂ»,3,4-trichloro-
	«alpha»,3,4-Trichlorotoluene
	Â«alphaÂ»,3,4-Trichlorotoluene
Inchi:	InChI=1S/C7H5Cl3/c8-4-5-1-2-6(9)7(10)3-5/h1-3H,4H2
InchiKey:	YZIFVWOCPGPNHB-UHFFFAOYSA-N
Formula:	C7H5Cl3
SMILES:	ClCc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	195.47
CAS:	102-47-6

Physical Properties

Property code	Value	Unit	Source
gf	65.42	kJ/mol	Joback Method
hf	-21.44	kJ/mol	Joback Method
hfus	19.74	kJ/mol	Joback Method
hvap	47.93	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.732		Crippen Method
mcvol	122.450	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
rinpol	1355.80		NIST Webbook
tb	514.20	K	NIST Webbook
tc	743.54	K	Joback Method
tf	309.87	K	Joback Method
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.02	J/mol×K	508.49	Joback Method

cpg	216.67	J/mol×K	547.67	Joback Method
cpg	224.73	J/mol×K	586.84	Joback Method
cpg	232.23	J/mol×K	626.02	Joback Method
cpg	239.19	J/mol×K	665.19	Joback Method
cpg	245.65	J/mol×K	704.37	Joback Method
cpg	251.62	J/mol×K	743.54	Joback Method
dvisc	0.0017070	Pa×s	309.87	Joback Method
dvisc	0.0010988	Pa×s	342.97	Joback Method
dvisc	0.0007643	Pa×s	376.08	Joback Method
dvisc	0.0005638	Pa×s	409.18	Joback Method
dvisc	0.0004353	Pa×s	442.28	Joback Method
dvisc	0.0003484	Pa×s	475.39	Joback Method
dvisc	0.0002870	Pa×s	508.49	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	396.20	K	1.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37973e+01
Coeff. B	-3.94803e+03
Coeff. C	-8.40840e+01
Temperature range (K), min.	376.32
Temperature range (K), max.	549.33

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=C102476&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

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