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

Other names:	1-Chloro-2-(chloromethyl)benzene
	2,alpha-Dichlorotoluene
	2,«alpha»-Dichlorotoluene
	2,Â«alphaÂ»-Dichlorotoluene
	2-Chlorobenzyl chloride
	NSC 8446
	Ortho-«alpha»-dichlorotoluene
	Ortho-Â«alphaÂ»-dichlorotoluene
	Toluene, o,«alpha»-dichloro-
	Toluene, o,Â«alphaÂ»-dichloro-
	alpha,o-Dichlorotoluene
	o,«alpha»-dichlorotoluene
	o,Â«alphaÂ»-dichlorotoluene
	o-Chlorobenzyl chloride
	«alpha»,2-Dichlorotoluene
	«alpha»,o-Dichlorotoluene
	Â«alphaÂ»,2-Dichlorotoluene
	Â«alphaÂ»,o-Dichlorotoluene
Inchi:	InChI=1S/C7H6Cl2/c8-5-6-3-1-2-4-7(6)9/h1-4H,5H2
InchiKey:	BASMANVIUSSIIM-UHFFFAOYSA-N
Formula:	C7H6Cl2
SMILES:	ClCc1ccccc1Cl
Mol. weight [g/mol]:	161.03
CAS:	611-19-8

Physical Properties

Property code	Value	Unit	Source
gf	86.98	kJ/mol	Joback Method
hf	5.77	kJ/mol	Joback Method
hfus	15.93	kJ/mol	Joback Method
hvap	42.88	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	3.079		Crippen Method
mcvol	110.210	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
tb	486.70	K	NIST Webbook
tc	694.10	K	Joback Method

tf	267.43	K	Joback Method
vc	0.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.80	J/mol×K	466.08	Joback Method
cpg	229.42	J/mol×K	656.09	Joback Method
cpg	222.08	J/mol×K	618.09	Joback Method
cpg	214.17	J/mol×K	580.09	Joback Method
cpg	205.68	J/mol×K	542.09	Joback Method
cpg	196.57	J/mol×K	504.08	Joback Method
cpg	236.24	J/mol×K	694.10	Joback Method
dvisc	0.0002875	Pa×s	466.08	Joback Method
dvisc	0.0003555	Pa×s	432.97	Joback Method
dvisc	0.0004554	Pa×s	399.86	Joback Method
dvisc	0.0006099	Pa×s	366.75	Joback Method
dvisc	0.0008657	Pa×s	333.65	Joback Method
dvisc	0.0013273	Pa×s	300.54	Joback Method
dvisc	0.0022622	Pa×s	267.43	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42356e+01
Coeff. B	-3.93626e+03
Coeff. C	-7.74120e+01
Temperature range (K), min.	359.62
Temperature range (K), max.	518.49

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C611198&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume