Benzene, (chloromethyl)-

Other names:	(chloromethyl)benzene
	.alpha.-chlorotoluene
	ALPHA-CHLOROTOLUENE
	Benzile (cloruro di)
	Benzylchlorid
	Benzylchloride
	Benzyle (chlorure de)
	C6H5CH2Cl
	Chloromethylbenzene
	Chlorophenylmethane
	Chlorure de benzyle
	NCI-C06360
	NSC 8043
	Phenylmethyl chloride
	Rcra waste number P028
	Toluene, «alpha»-chloro-
	Tolyl chloride
	UN 1738
	benzene, chloromethyl-
	benzyl chloride
	«alpha»-Chlorotoluene
	«alpha»-Chlortoluol
	«omega»-Chlorotoluene
Inchi:	InChI=1S/C7H7Cl/c8-6-7-4-2-1-3-5-7/h1-5H,6H2
InchiKey:	KCXMKQUNVWSEMD-UHFFFAOYSA-N
Formula:	C7H7Cl
SMILES:	ClCc1ccccc1
Mol. weight [g/mol]:	126.59
CAS:	100-44-7

Physical Properties

Property code	Value	Unit	Source
af	0.3025		Cheméo Relay (1.0)
gf	108.54	kJ/mol	Joback Method
hf	19.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-33.00 ± 3.00	kJ/mol	NIST Webbook

hfus	12.12	kJ/mol	Joback Method
hvap	51.00 ± 2.00	kJ/mol	NIST Webbook
hvap	50.10 ± 0.50	kJ/mol	NIST Webbook
hvap	49.90	kJ/mol	NIST Webbook
hvap	50.10 ± 0.30	kJ/mol	NIST Webbook
ie	9.29	eV	NIST Webbook
ie	9.10 ± 0.05	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
ie	9.14 ± 0.01	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
ie	9.14 ± 0.01	eV	NIST Webbook
ie	9.10 ± 0.02	eV	NIST Webbook
log10ws	-2.39		Estimated Solubility Method
log10ws	-2.39		Aqueous Solubility Prediction Method
logp	2.425		Crippen Method
mcvol	97.970	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=2)		KDB
nfpas	%!d(float64=1)		KDB
pc	3925.85	kPa	Joback Method
rinpol	1015.00		NIST Webbook
rinpol	996.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	977.90		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	985.60		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	986.00		NIST Webbook
ripol	1478.00		NIST Webbook
ripol	1478.00		NIST Webbook
ripol	1497.00		NIST Webbook
tb	452.50 ± 0.40	K	NIST Webbook
tb	452.50 ± 0.50	K	NIST Webbook
tb	452.15 ± 0.50	K	NIST Webbook
tb	447.00 ± 5.00	K	NIST Webbook
tb	452.00	K	NIST Webbook
tb	452.50	K	NIST Webbook

tb	452.50 ± 0.50	K	NIST Webbook
tb	452.15 ± 1.50	K	NIST Webbook
tb	452.15	K	KDB
tc	676.66	K	Cheméo Relay (1.0)
tf	233.95	K	KDB
tf	233.45 ± 0.40	K	NIST Webbook
tf	225.30 ± 0.50	K	NIST Webbook
tf	233.45 ± 0.40	K	NIST Webbook
tf	233.95 ± 0.30	K	NIST Webbook
tf	229.48	K	Aqueous Solubility Prediction Method
vc	0.350	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.08	J/mol×K	423.67	Joback Method
cpg	173.99	J/mol×K	460.28	Joback Method
cpg	184.20	J/mol×K	496.89	Joback Method
cpg	193.74	J/mol×K	533.50	Joback Method
cpg	202.64	J/mol×K	570.11	Joback Method
cpg	210.94	J/mol×K	606.72	Joback Method
cpg	218.66	J/mol×K	643.33	Joback Method
cpl	182.40	J/mol×K	298.50	NIST Webbook
dvisc	0.0031741	Pa×s	224.99	Joback Method
dvisc	0.0016248	Pa×s	258.10	Joback Method
dvisc	0.0009686	Pa×s	291.22	Joback Method
dvisc	0.0006417	Pa×s	324.33	Joback Method
dvisc	0.0004588	Pa×s	357.44	Joback Method
dvisc	0.0003473	Pa×s	390.56	Joback Method
dvisc	0.0002746	Pa×s	423.67	Joback Method
hfust	8.74	kJ/mol	230.00	NIST Webbook
hvapt	48.60	kJ/mol	355.00	NIST Webbook
hvapt	48.60	kJ/mol	374.00	NIST Webbook
rhol	1094.82	kg/m3	298.15	Excess Enthalpies of Chloroalkylbenzene + Alkylbenzene Mixtures

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41881e+01
Coeff. B	-3.68477e+03
Coeff. C	-6.69590e+01
Temperature range (K), min.	332.04
Temperature range (K), max.	482.07

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.79326e+01
Coeff. B	-7.14622e+03
Coeff. C	-4.52442e+00
Coeff. D	5.72779e-07
Temperature range (K), min.	234.15
Temperature range (K), max.	686.00

Sources

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Activity coefficient at infinite dilution measurements for organic solutes (polar and non-polar) in fatty compounds. Saturated fatty acids:	https://www.doi.org/10.1016/j.jct.2012.06.009
Activity coefficient at infinite dilution measurements for organic solutes (polar and non-polar) in fatty compounds. Part II: C18 fatty acids:	https://www.doi.org/10.1016/j.jct.2012.12.009
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1701.mol
Cheméo Relay (1.0, beta):	
Excess Enthalpies of Chloroalkylbenzene + Alkylbenzene Mixtures:	https://www.doi.org/10.1021/je7002447
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100447&Units=SI
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Cheméo Relay (1.0):	
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Determination of Henry's Law Constants Using Internal Standards with Benchmark Values:	https://www.doi.org/10.1021/je3010535
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1701

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume