Benzene, 1-(chloromethyl)-4-methyl-

Other names:	(4-Methylphenyl)methyl chloride
	1-(Chloromethyl)-4-methylbenzene
	1-Methyl-4-(chloromethyl)benzene
	4-(Chloromethyl)toluene
	4-Methylbenzyl chloride
	NSC 46590
	p-Chloromethyltoluene
	p-Methylbenzyl chloride
	p-Tolylmethyl chloride
	p-Xylene, alpha-chloro-
	p-Xylene, «alpha»-chloro-
	p-Xylene, Â«alphaÂ»-chloro-
	p-Xylyl chloride
	p-Xylyl-«alpha»-chloride
	p-Xylyl-Â«alphaÂ»-chloride
	«alpha»-Chloro-p-xylene
	Â«alphaÂ»-Chloro-p-xylene
Inchi:	InChI=1S/C8H9Cl/c1-7-2-4-8(6-9)5-3-7/h2-5H,6H2,1H3
InchiKey:	DMHZDOTYAVHSEH-UHFFFAOYSA-N
Formula:	C8H9Cl
SMILES:	Cc1ccc(CCl)cc1
Mol. weight [g/mol]:	140.61
CAS:	104-82-5

Physical Properties

Property code	Value	Unit	Source
gf	107.33	kJ/mol	Joback Method
hf	0.87	kJ/mol	Joback Method
hfus	14.32	kJ/mol	Joback Method
hvap	40.73	kJ/mol	Joback Method
ie	8.79 ± 0.03	eV	NIST Webbook
log10ws	-2.98		Crippen Method
logp	2.734		Crippen Method
mcvol	112.060	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
rinpol	1096.00		NIST Webbook
rinpol	1136.00		NIST Webbook

rinpol	1098.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1088.00		NIST Webbook
tb	474.20	K	NIST Webbook
tc	669.70	K	Joback Method
tf	248.78	K	Joback Method
vc	0.424	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.26	J/mol×K	451.53	Joback Method
cpg	213.97	J/mol×K	487.89	Joback Method
cpg	225.00	J/mol×K	524.25	Joback Method
cpg	235.38	J/mol×K	560.62	Joback Method
cpg	245.12	J/mol×K	596.98	Joback Method
cpg	254.26	J/mol×K	633.34	Joback Method
cpg	262.83	J/mol×K	669.70	Joback Method
dvisc	0.0022898	Pa×s	248.78	Joback Method
dvisc	0.0012755	Pa×s	282.57	Joback Method
dvisc	0.0008051	Pa×s	316.36	Joback Method
dvisc	0.0005554	Pa×s	350.15	Joback Method
dvisc	0.0004090	Pa×s	383.95	Joback Method
dvisc	0.0003165	Pa×s	417.74	Joback Method
dvisc	0.0002545	Pa×s	451.53	Joback Method
hvapt	44.90	kJ/mol	416.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42021e+01
Coeff. B	-3.84537e+03
Coeff. C	-7.29640e+01

Temperature range (K), min.	349.32
Temperature range (K), max.	505.48

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=C104825&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
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
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