Benzene, 1-(chloromethyl)-3-methyl-

Other names:	m-Xylene, «alpha»-chloro-
	«alpha»-Chloro-m-xylene
	m-(Chloromethyl)toluene
	m-Methylbenzyl chloride
	m-Xylyl chloride
	m-Xylyl-«alpha»-chloride
	3-(Chloromethyl)toluene
	3-Methylbenzyl chloride
	1-Chloromethyl-3-methylbenzene
	«alpha»-Chloro-meta-xylene
	alpha-Chloro-m-xylene
	1-Methyl-3-chloromethylbenzene
	NSC 76592
Inchi:	InChI=1S/C8H9Cl/c1-7-3-2-4-8(5-7)6-9/h2-5H,6H2,1H3
InchiKey:	LZBOHNCMCCSTJX-UHFFFAOYSA-N
Formula:	C8H9Cl
SMILES:	Cc1cccc(CCl)c1
Mol. weight [g/mol]:	140.61
CAS:	620-19-9

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	8.82 ± 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	1082.00		NIST Webbook
rinpol	1089.30		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1089.30		NIST Webbook
rinpol	1098.00		NIST Webbook
tb	468.70	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	254.26	J/mol×K	633.34	Joback Method
cpg	245.12	J/mol×K	596.98	Joback Method
cpg	235.38	J/mol×K	560.62	Joback Method
cpg	225.00	J/mol×K	524.25	Joback Method
cpg	213.97	J/mol×K	487.89	Joback Method
cpg	262.83	J/mol×K	669.70	Joback Method
dvisc	0.0002545	Pa×s	451.53	Joback Method
dvisc	0.0003165	Pa×s	417.74	Joback Method
dvisc	0.0004090	Pa×s	383.95	Joback Method
dvisc	0.0005554	Pa×s	350.15	Joback Method
dvisc	0.0008051	Pa×s	316.36	Joback Method
dvisc	0.0012755	Pa×s	282.57	Joback Method
dvisc	0.0022898	Pa×s	248.78	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C620199&Units=SI

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume