ALPHA-CHLORO-ORTHO-XYLENE

Other names:	1-(Chloromethyl)-2-methylbenzene
	2-(Chloromethyl)toluene
	2-Methylbenzyl chloride
	o-(Chloromethyl)toluene
	o-Methylbenzyl chloride
	o-Xylene, «alpha»-chloro-
	o-Xylyl chloride
	o-Xylyl-«alpha»-chloride
	«alpha»-Chloro-o-xylene
	«alpha»-Chloro-ortho-xylene
	«omega»-Chloro-o-xylene
Inchi:	InChI=1S/C8H9Cl/c1-7-4-2-3-5-8(7)6-9/h2-5H,6H2,1H3
InchiKey:	VQRBXYBBGHOGFT-UHFFFAOYSA-N
Formula:	C8H9Cl
SMILES:	Cc1ccccc1CCl
Mol. weight [g/mol]:	140.61
CAS:	552-45-4

Physical Properties

Property code	Value	Unit	Source
af	0.3453		Cheméo Relay (1.0)
gf	107.33	kJ/mol	Joback Method
hf	-18.53	kJ/mol	Cheméo Relay (1.0)
hfus	14.32	kJ/mol	Joback Method
hvap	53.68	kJ/mol	Cheméo Relay (1.0)
ie	8.89	eV	Cheméo Relay (1.0)
log10ws	-2.93		Cheméo Relay (1.0)
logp	2.734		Crippen Method
mcvol	112.060	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
rinpol	1098.00		NIST Webbook
rinpol	1105.00		NIST Webbook
tb	471.20	K	NIST Webbook
tc	699.94	K	Cheméo Relay (1.0)
tf	268.21	K	Cheméo Relay (1.0)
vc	0.401	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.26	J/mol×K	451.53	Joback Method
cpg	262.83	J/mol×K	669.70	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
dvisc	0.0005554	Pa×s	350.15	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	0.0022898	Pa×s	248.78	Joback Method
dvisc	0.0008051	Pa×s	316.36	Joback Method
dvisc	0.0012755	Pa×s	282.57	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41938e+01
Coeff. B	-3.82130e+03
Coeff. C	-7.21300e+01
Temperature range (K), min.	346.92
Temperature range (K), max.	502.34

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C552454&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume