

Benzenemethanol, 4-chloro-«alpha»-methyl-

Other names:	Benzyl alcohol, p-chloro-«alpha»-methyl-«alpha»-(p-Chlorophenyl)ethanol p-Chloro-«alpha»-methylbenzyl alcohol 1-(p-Chlorophenyl)ethanol 1-(4-Chlorophenyl)ethanol 1-p-Chlorophenylethyl alcohol 4-Chlorophenylmethylcarbinol 4-Chloro-alpha-methylbenzyl alcohol 4-chloro-«alpha»-methylbenzyl alcohol
Inchi:	InChI=1S/C8H9ClO/c1-6(10)7-2-4-8(9)5-3-7/h2-6,10H,1H3
InchiKey:	MVOSNPUNXINWAD-UHFFFAOYSA-N
Formula:	C8H9ClO
SMILES:	CC(O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	156.61
CAS:	3391-10-4

Physical Properties

Property code	Value	Unit	Source
gf	-31.93	kJ/mol	Joback Method
hf	-156.64	kJ/mol	Joback Method
hfus	14.89	kJ/mol	Joback Method
hvap	57.02	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.393		Crippen Method
mcvol	117.930	ml/mol	McGowan Method
pc	3872.29	kPa	Joback Method
rinpol	1226.30		NIST Webbook
rinpol	1226.30		NIST Webbook
tb	543.27	K	Joback Method
tc	751.23	K	Joback Method
tf	294.60	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.37	J/mol×K	543.27	Joback Method
cpg	291.43	J/mol×K	716.57	Joback Method
cpg	283.72	J/mol×K	681.91	Joback Method
cpg	275.49	J/mol×K	647.25	Joback Method
cpg	266.70	J/mol×K	612.59	Joback Method
cpg	257.34	J/mol×K	577.93	Joback Method
cpg	298.63	J/mol×K	751.23	Joback Method
dvisc	0.0001162	Pa×s	543.27	Joback Method
dvisc	0.0001827	Pa×s	501.82	Joback Method
dvisc	0.0003115	Pa×s	460.38	Joback Method
dvisc	0.0005903	Pa×s	418.94	Joback Method
dvisc	0.0012872	Pa×s	377.49	Joback Method
dvisc	0.0034019	Pa×s	336.05	Joback Method
dvisc	0.0118182	Pa×s	294.60	Joback Method

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=C3391104&Units=SI
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
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

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