

3-Chloro-4-methylbenzyl alcohol

Other names:	Benzenemethanol, 3-chloro-4-methyl-
Inchi:	InChI=1S/C8H9ClO/c1-6-2-3-7(5-10)4-8(6)9/h2-4,10H,5H2,1H3
InchiKey:	NLRJZTGNCBMNKS-UHFFFAOYSA-N
Formula:	C8H9ClO
SMILES:	Cc1ccc(CO)cc1Cl
Mol. weight [g/mol]:	156.61
CAS:	39652-32-9

Physical Properties

Property code	Value	Unit	Source
gf	-39.12	kJ/mol	Joback Method
hf	-162.83	kJ/mol	Joback Method
hfus	18.02	kJ/mol	Joback Method
hvap	58.07	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.141		Crippen Method
mcvol	117.930	ml/mol	McGowan Method
pc	3763.78	kPa	Joback Method
tb	548.69	K	Joback Method
tc	753.32	K	Joback Method
tf	322.12	K	Joback Method
vc	0.444	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.18	J/mol×K	548.69	Joback Method
cpg	255.58	J/mol×K	582.80	Joback Method
cpg	264.46	J/mol×K	616.90	Joback Method
cpg	272.84	J/mol×K	651.01	Joback Method
cpg	280.75	J/mol×K	685.11	Joback Method
cpg	288.19	J/mol×K	719.22	Joback Method
cpg	295.19	J/mol×K	753.32	Joback Method
dvisc	0.0047515	Paxs	322.12	Joback Method

dvisc	0.0018562	Paxs	359.88	Joback Method
dvisc	0.0008668	Paxs	397.64	Joback Method
dvisc	0.0004620	Paxs	435.40	Joback Method
dvisc	0.0002722	Paxs	473.17	Joback Method
dvisc	0.0001735	Paxs	510.93	Joback Method
dvisc	0.0001176	Paxs	548.69	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	410.50 ± 0.50	K	0.90	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39652329&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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