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	m3/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	Pa×s	322.12	Joback Method

dvisc	0.0018562	Pa×s	359.88	Joback Method
dvisc	0.0008668	Pa×s	397.64	Joback Method
dvisc	0.0004620	Pa×s	435.40	Joback Method
dvisc	0.0002722	Pa×s	473.17	Joback Method
dvisc	0.0001735	Pa×s	510.93	Joback Method
dvisc	0.0001176	Pa×s	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

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=C39652329&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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