3-Chlorobenzyl alcohol

Other names: m-Chlorobenzyl alcohol
Benzenemethanol, 3-chloro-
Inchi: InChI=1S/C7H7ClO/c8-7-3-1-2-6(4-7)5-9/h1-4,9H,5H2
InchiKey: ZSRDNPVYGSFUMD-UHFFFAOYSA-N
Formula: C7H7ClO
SMILES: OCc1cccc(Cl)c1
Mol. weight [g/mol]: 142.58
CAS: 873-63-2

Physical Properties

Property code	Value	Unit	Source
gf	-37.91	kJ/mol	Joback Method
hf	-130.72	kJ/mol	Joback Method
hfus	15.82	kJ/mol	Joback Method
hvap	55.18	kJ/mol	Joback Method
ie	8.51	eV	NIST Webbook
log10ws	-2.30		Crippen Method
logp	1.832		Crippen Method
mcvol	103.840	ml/mol	McGowan Method
pc	4333.96	kPa	Joback Method
tb	510.20	K	NIST Webbook
tc	727.48	K	Joback Method
tf	298.33	K	Joback Method
vc	0.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.63	J/mol×K	520.83	Joback Method
cpg	242.77	J/mol×K	693.04	Joback Method
cpg	236.09	J/mol×K	658.60	Joback Method
cpg	228.96	J/mol×K	624.16	Joback Method
cpg	221.36	J/mol×K	589.71	Joback Method
cpg	213.25	J/mol×K	555.27	Joback Method

cpg	249.01	J/mol×K	727.48	Joback Method
dvisc	0.0001451	Pa×s	520.83	Joback Method
dvisc	0.0002205	Pa×s	483.75	Joback Method
dvisc	0.0003591	Pa×s	446.66	Joback Method
dvisc	0.0006389	Pa×s	409.58	Joback Method
dvisc	0.0012750	Pa×s	372.50	Joback Method
dvisc	0.0029645	Pa×s	335.41	Joback Method
dvisc	0.0085009	Pa×s	298.33	Joback Method

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=C873632&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
ie:	Ionization energy
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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