

4-Chlorobenzyl alcohol

Other names:	p-Chlorobenzyl alcohol Benzenemethanol, 4-chloro- Benzyl alcohol, p-chloro- 4-chlorobenzyl alcohol
Inchi:	InChI=1S/C7H7ClO/c8-7-3-1-6(5-9)2-4-7/h1-4,9H,5H2
InchiKey:	PTHGDVPCZKZKR-UHFFFAOYSA-N
Formula:	C7H7ClO
SMILES:	OCc1ccc(Cl)cc1
Mol. weight [g/mol]:	142.58
CAS:	873-76-7

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	8.58	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	508.20	K	NIST Webbook
tc	727.48	K	Joback Method
tf	298.33	K	Joback Method
vc	0.388	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

cpg	236.09	J/mol×K	658.60	Joback Method
cpg	242.77	J/mol×K	693.04	Joback Method
cpg	249.01	J/mol×K	727.48	Joback Method
dvisc	0.0085009	Paxs	298.33	Joback Method
dvisc	0.0029645	Paxs	335.41	Joback Method
dvisc	0.0012750	Paxs	372.50	Joback Method
dvisc	0.0006389	Paxs	409.58	Joback Method
dvisc	0.0003591	Paxs	446.66	Joback Method
dvisc	0.0002205	Paxs	483.75	Joback Method
dvisc	0.0001451	Paxs	520.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C873767&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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