

4-Chlorophenyl methyl carbinol

Other names:	Benzeneethanol, 4-chloro-p-chlorophenethylic alcohol
Inchi:	InChI=1S/C8H9ClO/c9-8-3-1-7(2-4-8)5-6-10/h1-4,10H,5-6H2
InchiKey:	HZFRKZWBVUJYDA-UHFFFAOYSA-N
Formula:	C8H9ClO
SMILES:	OCCc1ccc(Cl)cc1
Mol. weight [g/mol]:	156.61
CAS:	1875-88-3

Physical Properties

Property code	Value	Unit	Source
gf	-29.49	kJ/mol	Joback Method
hf	-151.36	kJ/mol	Joback Method
hfus	18.41	kJ/mol	Joback Method
hvap	57.40	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	1.875		Crippen Method
mcvol	117.930	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
tb	532.20	K	NIST Webbook
tc	747.28	K	Joback Method
tf	309.60	K	Joback Method
vc	0.444	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.09	J/molxK	747.28	Joback Method
cpg	246.99	J/molxK	543.71	Joback Method
cpg	256.68	J/molxK	577.64	Joback Method
cpg	265.80	J/molxK	611.57	Joback Method
cpg	274.38	J/molxK	645.50	Joback Method
cpg	282.44	J/molxK	679.42	Joback Method
cpg	290.00	J/molxK	713.35	Joback Method

dvisc	0.0001234	Paxs	543.71	Joback Method
dvisc	0.0073323	Paxs	309.60	Joback Method
dvisc	0.0025361	Paxs	348.62	Joback Method
dvisc	0.0010862	Paxs	387.64	Joback Method
dvisc	0.0005433	Paxs	426.66	Joback Method
dvisc	0.0003052	Paxs	465.67	Joback Method
dvisc	0.0001874	Paxs	504.69	Joback Method
hvapt	59.30	kJ/mol	549.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	383.20	K	0.07	NIST Webbook

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1875883&Units=SI

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
hvapt:	Enthalpy of vaporization at a given temperature
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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