

P-CHLOROPHENETHYL ALCOHOL

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

Physical Properties

Property code	Value	Unit	Source
hf	-170.44	kJ/mol	Cheméo Relay (1.0)
hfus	18.41	kJ/mol	Joback Method
hvap	77.67	kJ/mol	Cheméo Relay (1.0)
ie	8.75	eV	Cheméo Relay (1.0)
log10ws	-1.76		Cheméo Relay (1.0)
logp	1.875		Crippen Method
mcvol	117.930	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
tb	532.20	K	NIST Webbook
tf	290.22	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.00	J/mol×K	713.35	Joback Method
cpg	297.09	J/mol×K	747.28	Joback Method
cpg	256.68	J/mol×K	577.64	Joback Method
cpg	265.80	J/mol×K	611.57	Joback Method
cpg	274.38	J/mol×K	645.50	Joback Method
cpg	282.44	J/mol×K	679.42	Joback Method
cpg	246.99	J/mol×K	543.71	Joback Method
dvisc	0.0010862	Pa×s	387.64	Joback Method
dvisc	0.0025361	Pa×s	348.62	Joback Method
dvisc	0.0073323	Pa×s	309.60	Joback Method

dvisc	0.0005433	Pa×s	426.66	Joback Method
dvisc	0.0003052	Pa×s	465.67	Joback Method
dvisc	0.0001874	Pa×s	504.69	Joback Method
dvisc	0.0001234	Pa×s	543.71	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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1875883&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
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

tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point

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