Benzeneethanol, 3-chloro-

Other names:	Phenethyl alcohol, m-chloro-
	2-(3-Chlorophenyl)ethanol
	m-Chlorophenethyl alcohol
	m-chlorophenethylic alcohol
Inchi:	InChI=1S/C8H9ClO/c9-8-3-1-2-7(6-8)4-5-10/h1-3,6,10H,4-5H2
InchiKey:	NDWAVJKRSASRPH-UHFFFAOYSA-N
Formula:	C8H9ClO
SMILES:	OCCc1cccc(Cl)c1
Mol. weight [g/mol]:	156.61
CAS:	5182-44-5

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	543.71	K	Joback Method
tc	747.28	K	Joback Method
tf	309.60	K	Joback Method
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.99	J/mol×K	543.71	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	290.00	J/mol×K	713.35	Joback Method
cpg	297.09	J/mol×K	747.28	Joback Method
dvisc	0.0073323	Pa×s	309.60	Joback Method
dvisc	0.0025361	Pa×s	348.62	Joback Method
dvisc	0.0010862	Pa×s	387.64	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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.20	K	1.70	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C5182445&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
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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