O-CHLOROPHENETHYL ALCOHOL

Other names: o-Chlorophenylmethylcarbinol
Benzeneethanol, 2-chloro-
o-chlorophenethylic alcohol
Inchi: InChI=1S/C8H9ClO/c9-8-4-2-1-3-7(8)5-6-10/h1-4,10H,5-6H2
InchiKey: IWNHTCBFRSCBQK-UHFFFAOYSA-N
Formula: C8H9ClO
SMILES: OCCc1ccccc1Cl
Mol. weight [g/mol]: 156.61

Physical Properties

Property code	Value	Unit	Source
af	0.6153		Cheméo Relay (1.0)
gf	-29.49	kJ/mol	Joback Method
hf	-172.41	kJ/mol	Cheméo Relay (1.0)
hfus	18.41	kJ/mol	Joback Method
hvap	75.33	kJ/mol	Cheméo Relay (1.0)
ie	8.90	eV	Cheméo Relay (1.0)
log10ws	-1.54		Cheméo Relay (1.0)
logp	1.875		Crippen Method
mcvol	117.930	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
tb	530.51	K	Cheméo Relay (1.0)
tc	771.51	K	Cheméo Relay (1.0)
tf	272.36	K	Cheméo Relay (1.0)
vc	0.413	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.99	J/mol×K	543.71	Joback Method
cpg	297.09	J/mol×K	747.28	Joback Method
cpg	290.00	J/mol×K	713.35	Joback Method
cpg	282.44	J/mol×K	679.42	Joback Method
cpg	274.38	J/mol×K	645.50	Joback Method

cpg	265.80	J/mol×K	611.57	Joback Method
cpg	256.68	J/mol×K	577.64	Joback Method
dvisc	0.0005433	Pa×s	426.66	Joback Method
dvisc	0.0001234	Pa×s	543.71	Joback Method
dvisc	0.0001874	Pa×s	504.69	Joback Method
dvisc	0.0003052	Pa×s	465.67	Joback Method
dvisc	0.0073323	Pa×s	309.60	Joback Method
dvisc	0.0010862	Pa×s	387.64	Joback Method
dvisc	0.0025361	Pa×s	348.62	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	357.70	K	0.40	NIST Webbook

Sources

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=C19819955&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume