PHENOL, 2-CHLORO-6-[2-PROPENYL]-

Other names: Phenol, 2-chloro-6-[2-propenyl]-
Inchi: InChI=1S/C9H9ClO/c1-2-4-7-5-3-6-8(10)9(7)11/h2-3,5-6,11H,1,4H2
InchiKey: UPEBXJHGPMUFKU-UHFFFAOYSA-N
Formula: C9H9ClO
SMILES: C=CCc1cccc(Cl)c1O
Mol. weight [g/mol]: 168.62

Physical Properties

Property code	Value	Unit	Source
hf	-76.81	kJ/mol	Cheméo Relay (1.0)
hfus	21.42	kJ/mol	Joback Method
hvap	65.09	kJ/mol	Cheméo Relay (1.0)
ie	8.33	eV	Cheméo Relay (1.0)
log10ws	-2.21		Cheméo Relay (1.0)
logp	2.774		Crippen Method
mcvol	127.720	ml/mol	McGowan Method
tb	485.81	K	Cheméo Relay (1.0)
tf	280.21	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.45	J/mol×K	551.71	Joback Method
cpg	283.29	J/mol×K	590.56	Joback Method
cpg	293.30	J/mol×K	629.42	Joback Method
cpg	302.56	J/mol×K	668.27	Joback Method
cpg	311.17	J/mol×K	707.12	Joback Method
cpg	319.22	J/mol×K	745.98	Joback Method
cpg	326.79	J/mol×K	784.83	Joback Method
dvisc	0.0016729	Pa×s	370.01	Joback Method
dvisc	0.0007757	Pa×s	400.29	Joback Method
dvisc	0.0004007	Pa×s	430.58	Joback Method
dvisc	0.0002258	Pa×s	460.86	Joback Method
dvisc	0.0001366	Pa×s	491.14	Joback Method

dvisc	0.0000875	Pa×s	521.43	Joback Method
dvisc	0.0000589	Pa×s	551.71	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5348072&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
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point