3-Chloro-4-methylphenol

Other names: p-Cresol, 3-chloro-
3-Chloro-p-cresol
3-Chloro-4-methylphenol
Inchi: InChI=1S/C7H7ClO/c1-5-2-3-6(9)4-7(5)8/h2-4,9H,1H3
InchiKey: VQZRLBWPEHFGCD-UHFFFAOYSA-N
Formula: C7H7ClO
SMILES: Cc1ccc(O)cc1Cl
Mol. weight [g/mol]: 142.59

Physical Properties

Property code	Value	Unit	Source
hf	-160.85	kJ/mol	Cheméo Relay (1.0)
hfus	17.52	kJ/mol	Joback Method
hvap	69.37	kJ/mol	Cheméo Relay (1.0)
ie	8.53	eV	Cheméo Relay (1.0)
log10ws	-1.63		Cheméo Relay (1.0)
logp	2.354		Crippen Method
mcvol	103.840	ml/mol	McGowan Method
pc	4678.49	kPa	Joback Method
tb	501.20	K	NIST Webbook
tc	751.48	K	Cheméo Relay (1.0)
tf	325.61	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.51	J/mol×K	509.27	Joback Method
cpg	215.97	J/mol×K	548.75	Joback Method
cpg	224.67	J/mol×K	588.22	Joback Method
cpg	232.68	J/mol×K	627.70	Joback Method
cpg	240.10	J/mol×K	667.17	Joback Method
cpg	246.99	J/mol×K	706.65	Joback Method
cpg	253.43	J/mol×K	746.12	Joback Method
dvisc	0.0023623	Pa×s	349.23	Joback Method

dvisc	0.0011285	Pa×s	375.90	Joback Method
dvisc	0.0005946	Pa×s	402.58	Joback Method
dvisc	0.0003392	Pa×s	429.25	Joback Method
dvisc	0.0002067	Pa×s	455.92	Joback Method
dvisc	0.0001330	Pa×s	482.60	Joback Method
dvisc	0.0000896	Pa×s	509.27	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C615623&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):

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
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point