

Phenol, 2-chloro-6-methyl-

Other names:	o-Cresol, 6-chloro- 2-Chloro-6-methylphenol 2-Methyl-6-chlorophenol 6-Chloro-o-cresol
Inchi:	InChI=1S/C7H7ClO/c1-5-3-2-4-6(8)7(5)9/h2-4,9H,1H3
InchiKey:	YPNZJHFXFVLXSE-UHFFFAOYSA-N
Formula:	C7H7ClO
SMILES:	Cc1cccc(Cl)c1O
Mol. weight [g/mol]:	142.58
CAS:	87-64-9

Physical Properties

Property code	Value	Unit	Source
gf	-55.71	kJ/mol	Joback Method
hf	-155.80	kJ/mol	Joback Method
hfus	17.52	kJ/mol	Joback Method
hvap	51.51	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	2.354		Crippen Method
mcvol	103.840	ml/mol	McGowan Method
pc	4678.49	kPa	Joback Method
tb	509.27	K	Joback Method
tc	746.12	K	Joback Method
tf	349.23	K	Joback Method
vc	0.335	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.51	J/molxK	509.27	Joback Method
cpg	246.99	J/molxK	706.65	Joback Method
cpg	240.10	J/molxK	667.17	Joback Method
cpg	232.68	J/molxK	627.70	Joback Method
cpg	224.67	J/molxK	588.22	Joback Method

cpg	215.97	J/molxK	548.75	Joback Method
cpg	253.43	J/molxK	746.12	Joback Method
dvisc	0.0000896	Paxs	509.27	Joback Method
dvisc	0.0001330	Paxs	482.60	Joback Method
dvisc	0.0002067	Paxs	455.92	Joback Method
dvisc	0.0003392	Paxs	429.25	Joback Method
dvisc	0.0005946	Paxs	402.58	Joback Method
dvisc	0.0011285	Paxs	375.90	Joback Method
dvisc	0.0023623	Paxs	349.23	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	461.70	K	98.70	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C87649&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
mvol:	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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