

o-Cresol, 3,4,6-trichloro-

Other names:	3,4,6-Trichloro-O-cresol
Inchi:	InChI=1S/C7H5Cl3O/c1-3-6(10)4(8)2-5(9)7(3)11/h2,11H,1H3
InchiKey:	IAGVLEMVUDJCJS-UHFFFAOYSA-N
Formula:	C7H5Cl3O
SMILES:	Cc1c(O)c(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	211.47
CAS:	643-14-1

Physical Properties

Property code	Value	Unit	Source
gf	-98.83	kJ/mol	Joback Method
hf	-210.22	kJ/mol	Joback Method
hfus	25.13	kJ/mol	Joback Method
hvap	61.61	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.661		Crippen Method
mcvol	128.320	ml/mol	McGowan Method
pc	4077.71	kPa	Joback Method
tb	594.09	K	Joback Method
tc	841.74	K	Joback Method
tf	434.11	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.92	J/mol×K	594.09	Joback Method
cpg	251.08	J/mol×K	635.37	Joback Method
cpg	257.71	J/mol×K	676.64	Joback Method
cpg	263.89	J/mol×K	717.92	Joback Method
cpg	269.69	J/mol×K	759.19	Joback Method
cpg	275.19	J/mol×K	800.47	Joback Method
cpg	280.47	J/mol×K	841.74	Joback Method
dvisc	0.0005333	Pa×s	434.11	Joback Method

dvisc	0.0003181	Pa×s	460.77	Joback Method
dvisc	0.0002008	Pa×s	487.44	Joback Method
dvisc	0.0001329	Pa×s	514.10	Joback Method
dvisc	0.0000917	Pa×s	540.76	Joback Method
dvisc	0.0000655	Pa×s	567.43	Joback Method
dvisc	0.0000482	Pa×s	594.09	Joback Method

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=C643141&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/63-678-0/o-Cresol-3-4-6-trichloro.pdf>

Generated by Cheméo on 2025-12-05 11:31:28.959084703 +0000 UTC m=+4682486.489125357.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.