

1,2-Benzenediol, 3,4,5-trichloro-

Other names:	3,4,5-Trichloro-benzene-1,2-diol 3,4,5-Trichloro-1,2-benzenediol
Inchi:	InChI=1S/C6H3Cl3O2/c7-2-1-3(10)6(11)5(9)4(2)8/h1,10-11H
InchiKey:	FUTDYIMYZIMPBJ-UHFFFAOYSA-N
Formula:	C6H3Cl3O2
SMILES:	Oc1cc(Cl)c(Cl)c(Cl)c1O
Mol. weight [g/mol]:	213.45
CAS:	56961-20-7

Physical Properties

Property code	Value	Unit	Source
gf	-252.24	kJ/mol	Joback Method
hf	-355.42	kJ/mol	Joback Method
hfus	28.72	kJ/mol	Joback Method
hvap	71.73	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	3.058		Crippen Method
mcvol	120.100	ml/mol	McGowan Method
pc	5862.92	kPa	Joback Method
tb	646.85	K	Joback Method
tc	908.14	K	Joback Method
tf	522.04	K	Joback Method
vc	0.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.68	J/mol×K	646.85	Joback Method
cpg	239.58	J/mol×K	690.40	Joback Method
cpg	244.13	J/mol×K	733.95	Joback Method
cpg	248.49	J/mol×K	777.49	Joback Method
cpg	252.83	J/mol×K	821.04	Joback Method
cpg	257.32	J/mol×K	864.59	Joback Method
cpg	262.10	J/mol×K	908.14	Joback Method

dvisc	0.0000504	Pa×s	522.04	Joback Method
dvisc	0.0000317	Pa×s	542.84	Joback Method
dvisc	0.0000206	Pa×s	563.64	Joback Method
dvisc	0.0000138	Pa×s	584.45	Joback Method
dvisc	0.0000095	Pa×s	605.25	Joback Method
dvisc	0.0000067	Pa×s	626.05	Joback Method
dvisc	0.0000048	Pa×s	646.85	Joback Method
hvapt	79.30	kJ/mol	308.00	NIST Webbook

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=C56961207&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
hvapt:	Enthalpy of vaporization at a given temperature
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

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