3,4,5-TRICHLORO-BENZENE-1,2-DIOL

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

Physical Properties

Property code	Value	Unit	Source
hf	-329.42	kJ/mol	Cheméo Relay (1.0)
hfus	28.72	kJ/mol	Joback Method
hvap	97.80	kJ/mol	Cheméo Relay (1.0)
ie	8.55	eV	Cheméo Relay (1.0)
log10ws	-2.63		Cheméo Relay (1.0)
logp	3.058		Crippen Method
mcvol	120.100	ml/mol	McGowan Method
tb	553.36	K	Cheméo Relay (1.0)
tf	393.94	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.68	J/mol×K	646.85	Joback Method
cpg	262.10	J/mol×K	908.14	Joback Method
cpg	257.32	J/mol×K	864.59	Joback Method
cpg	252.83	J/mol×K	821.04	Joback Method
cpg	248.49	J/mol×K	777.49	Joback Method
cpg	244.13	J/mol×K	733.95	Joback Method
cpg	239.58	J/mol×K	690.40	Joback Method
dvisc	0.0000138	Pa×s	584.45	Joback Method
dvisc	0.0000048	Pa×s	646.85	Joback Method
dvisc	0.0000067	Pa×s	626.05	Joback Method
dvisc	0.0000095	Pa×s	605.25	Joback Method

dvisc	0.0000504	Pa×s	522.04	Joback Method
dvisc	0.0000206	Pa×s	563.64	Joback Method
dvisc	0.0000317	Pa×s	542.84	Joback Method
hvapt	79.30	kJ/mol	308.00	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C56961207&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
hvapt: Enthalpy of vaporization at a given temperature
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