3,5-DICHLORO-BENZENE-1,2-DIOL

Other names: 3,5-Dichloro-benzene-1,2-diol
3,5-dichlorocatechol
Inchi: InChI=1S/C6H4Cl2O2/c7-3-1-4(8)6(10)5(9)2-3/h1-2,9-10H
InchiKey: XSXYVLIPQMXCBV-UHFFFAOYSA-N
Formula: C6H4Cl2O2
SMILES: Oc1cc(Cl)cc(Cl)c1O
Mol. weight [g/mol]: 179.00

Physical Properties

Property code	Value	Unit	Source
hf	-310.22	kJ/mol	Cheméo Relay (1.0)
hfus	24.91	kJ/mol	Joback Method
hvap	89.77	kJ/mol	Cheméo Relay (1.0)
ie	8.57	eV	Cheméo Relay (1.0)
log10ws	-1.69		Cheméo Relay (1.0)
logp	2.405		Crippen Method
mcvol	107.860	ml/mol	McGowan Method
tb	525.60	K	Cheméo Relay (1.0)
tf	367.02	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.56	J/mol×K	604.44	Joback Method
cpg	226.43	J/mol×K	647.35	Joback Method
cpg	231.76	J/mol×K	690.27	Joback Method
cpg	236.70	J/mol×K	733.18	Joback Method
cpg	241.40	J/mol×K	776.09	Joback Method
cpg	246.05	J/mol×K	819.00	Joback Method
cpg	250.80	J/mol×K	861.92	Joback Method
dvisc	0.0001179	Pa×s	479.60	Joback Method
dvisc	0.0000687	Pa×s	500.41	Joback Method
dvisc	0.0000418	Pa×s	521.21	Joback Method
dvisc	0.0000264	Pa×s	542.02	Joback Method

dvisc	0.0000173	Pa×s	562.83	Joback Method
dvisc	0.0000117	Pa×s	583.63	Joback Method
dvisc	0.0000081	Pa×s	604.44	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13673922&Units=SI

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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point