cis-1,2-Cyclohexanediol

Other names: 1,2-Cyclohexanediol, (Z)-
1,2-cyclohexanediol, cis-
Grandidentol
cis-1,2-Dihydroxycyclohexane
Inchi: InChI=1S/C6H12O2/c7-5-3-1-2-4-6(5)8/h5-8H,1-4H2/t5-,6+
InchiKey: PFURGBBHAOXLIO-OLQVQODUSA-N
Formula: C6H12O2
SMILES: OC1CCCCC1O
Mol. weight [g/mol]: 116.16
CAS: 1792-81-0

Physical Properties

Property code	Value	Unit	Source
chs	-3516.00 ± 0.40	kJ/mol	NIST Webbook
chs	-3521.00	kJ/mol	NIST Webbook
gf	-257.26	kJ/mol	Joback Method
hf	-437.65	kJ/mol	Joback Method
hfus	12.38	kJ/mol	Joback Method
hvap	62.43	kJ/mol	Joback Method
log10ws	-0.98		Crippen Method
logp	0.282		Crippen Method
mcvol	96.280	ml/mol	McGowan Method
pc	4835.95	kPa	Joback Method
tb	535.92	K	Joback Method
tc	720.36	K	Joback Method
tf	371.15 ± 1.00	K	NIST Webbook
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.23	J/mol×K	535.92	Joback Method
cpg	300.56	J/mol×K	720.36	Joback Method
cpg	291.95	J/mol×K	689.62	Joback Method

cpg	273.22	J/mol×K	628.14	Joback Method
cpg	252.43	J/mol×K	566.66	Joback Method
cpg	263.09	J/mol×K	597.40	Joback Method
cpg	282.84	J/mol×K	658.88	Joback Method
cps	191.80	J/mol×K	348.10	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	180.80	J/mol×K	333.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	175.00	J/mol×K	323.30	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	171.90	J/mol×K	316.00	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	177.20	J/mol×K	328.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	192.50	J/mol×K	350.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	184.30	J/mol×K	339.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	186.20	J/mol×K	344.10	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	89.60	J/mol×K	174.30	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	92.70	J/mol×K	185.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	100.00	J/mol×K	193.10	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K

cps	101.10	J/mol×K	202.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	111.00	J/mol×K	215.90	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	121.10	J/mol×K	230.10	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	168.00	J/mol×K	308.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	134.90	J/mol×K	259.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	138.20	J/mol×K	266.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	141.40	J/mol×K	273.10	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	148.80	J/mol×K	278.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	151.10	J/mol×K	283.00	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	152.00	J/mol×K	288.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	154.20	J/mol×K	288.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	157.80	J/mol×K	293.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K

cps	157.60	J/mol×K	293.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	160.40	J/mol×K	298.10	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	162.00	J/mol×K	300.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	163.90	J/mol×K	300.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	127.30	J/mol×K	248.10	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	166.40	J/mol×K	308.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	190.00	J/mol×K	346.30	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
dvisc	0.0029585	Pa×s	366.75	Joback Method
dvisc	0.0009076	Pa×s	409.04	Joback Method
dvisc	0.0000802	Pa×s	535.92	Joback Method
dvisc	0.0003475	Pa×s	451.33	Joback Method
dvisc	0.0001568	Pa×s	493.63	Joback Method
dvisc	0.0131225	Pa×s	324.45	Joback Method
dvisc	0.0909733	Pa×s	282.16	Joback Method
hfust	20.27	kJ/mol	373.20	NIST Webbook
hfust	3.30	kJ/mol	371.60	NIST Webbook
hfust	3.32	kJ/mol	371.60	NIST Webbook
hfust	19.89	kJ/mol	360.40	NIST Webbook
hfust	3.32	kJ/mol	371.60	NIST Webbook
hsubt	43.70	kJ/mol	304.50	NIST Webbook
sfust	55.19	J/mol×K	360.40	NIST Webbook
sfust	8.93	J/mol×K	371.60	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K:	https://www.doi.org/10.1021/je800047t
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=C1792810&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase 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
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume