1,4-Cyclohexanediol, trans-

Other names: 1,4-Cyclohexanediol, (E)-
trans-1,4-Dihydroxycyclohexane
trans-1,4-cyclohexanediol
Inchi: InChI=1S/C6H12O2/c7-5-1-2-6(8)4-3-5/h5-8H,1-4H2/t5-,6-
InchiKey: VKONPUDBRVKQLM-IZLXSQMJSA-N
Formula: C6H12O2
SMILES: OC1CCC(O)CC1
Mol. weight [g/mol]: 116.16
CAS: 6995-79-5

Physical Properties

Property code	Value	Unit	Source
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	383.15 ± 2.00	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	263.09	J/mol×K	597.40	Joback Method
cpg	273.22	J/mol×K	628.14	Joback Method
cpg	282.84	J/mol×K	658.88	Joback Method
cpg	291.95	J/mol×K	689.62	Joback Method
cpg	300.56	J/mol×K	720.36	Joback Method

cpg	252.43	J/mol×K	566.66	Joback Method
cps	127.30	J/mol×K	230.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	135.40	J/mol×K	238.30	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	142.20	J/mol×K	258.30	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	145.60	J/mol×K	273.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	148.80	J/mol×K	278.10	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	150.60	J/mol×K	278.10	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	149.00	J/mol×K	278.10	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	151.00	J/mol×K	283.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	151.10	J/mol×K	283.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	154.00	J/mol×K	288.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	124.60	J/mol×K	222.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	157.40	J/mol×K	293.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K

cps	167.00	J/mol×K	303.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	168.10	J/mol×K	308.10	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	169.90	J/mol×K	308.10	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	121.00	J/mol×K	215.00	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	174.00	J/mol×K	323.30	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	177.40	J/mol×K	333.10	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	181.40	J/mol×K	343.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	183.90	J/mol×K	343.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	187.10	J/mol×K	353.10	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	190.50	J/mol×K	363.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	198.00	J/mol×K	373.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	115.60	J/mol×K	206.90	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K

cps	115.40	J/mol×K	198.90	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	109.50	J/mol×K	189.10	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	105.60	J/mol×K	183.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	156.40	J/mol×K	293.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	173.00	J/mol×K	313.20	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
cps	100.60	J/mol×K	176.50	molar heat capacities of 1,2-cyclohexanediol isomers from (173 to 428) K
dvisc	0.0001568	Pa×s	493.63	Joback Method
dvisc	0.0003475	Pa×s	451.33	Joback Method
dvisc	0.0009076	Pa×s	409.04	Joback Method
dvisc	0.0029585	Pa×s	366.75	Joback Method
dvisc	0.0131225	Pa×s	324.45	Joback Method
dvisc	0.0909733	Pa×s	282.16	Joback Method
dvisc	0.0000802	Pa×s	535.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6995795&Units=SI
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

Legend

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
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