1,4-Cyclohexanediol

Other names:	Quinitol
	1,4-Cyclohexanediol,c&t
	1,4-Cyclohexanediol cis+trans
	Quinitol,c&t
	cyclohexane-1,4-diol
Inchi:	InChI=1S/C6H12O2/c7-5-1-2-6(8)4-3-5/h5-8H,1-4H2
InchiKey:	VKONPUDBRVKQLM-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	OC1CCC(O)CC1
Mol. weight [g/mol]:	116.16
CAS:	556-48-9

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	282.16	K	Joback Method
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	252.43	J/mol×K	566.66	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
dvisc	0.0909733	Pa×s	282.16	Joback Method
dvisc	0.0131225	Pa×s	324.45	Joback Method
dvisc	0.0029585	Pa×s	366.75	Joback Method
dvisc	0.0009076	Pa×s	409.04	Joback Method
dvisc	0.0003475	Pa×s	451.33	Joback Method
dvisc	0.0001568	Pa×s	493.63	Joback Method
dvisc	0.0000802	Pa×s	535.92	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	423.20	K	2.70	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=C556489&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume