

1,4-Cyclohexanedimethanol, trans-

Other names:	trans-1,4-Cyclohexanedimethanol (trans-4-Hydroxymethylcyclohexyl)methanol Cyclohex-1,4-ylenedimethanol, trans trans-1,4-Bis(hydroxymethyl)cyclohexane CHDM, trans isomer trans-CHDM
Inchi:	InChI=1S/C8H16O2/c9-5-7-1-2-8(6-10)4-3-7/h7-10H,1-6H2/t7-,8-
InchiKey:	YIMQCDZDWXUDCA-ZKCHVHJHSA-N
Formula:	C8H16O2
SMILES:	OCC1CCC(CO)CC1
Mol. weight [g/mol]:	144.21
CAS:	3236-48-4

Physical Properties

Property code	Value	Unit	Source
gf	-240.42	kJ/mol	Joback Method
hf	-478.93	kJ/mol	Joback Method
hfus	17.56	kJ/mol	Joback Method
hvap	66.88	kJ/mol	Joback Method
log10ws	-1.11		Crippen Method
logp	0.777		Crippen Method
mcvol	124.460	ml/mol	McGowan Method
pc	3763.78	kPa	Joback Method
tb	581.68	K	Joback Method
tc	762.42	K	Joback Method
tf	304.70	K	Joback Method
vc	0.454	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.28	J/mol×K	581.68	Joback Method
cpg	347.06	J/mol×K	611.80	Joback Method
cpg	359.21	J/mol×K	641.93	Joback Method

cpg	370.76	J/molxK	672.05	Joback Method
cpg	381.72	J/molxK	702.18	Joback Method
cpg	392.09	J/molxK	732.30	Joback Method
cpg	401.91	J/molxK	762.42	Joback Method
dvisc	0.0469058	Paxs	304.70	Joback Method
dvisc	0.0070785	Paxs	350.86	Joback Method
dvisc	0.0016582	Paxs	397.03	Joback Method
dvisc	0.0005256	Paxs	443.19	Joback Method
dvisc	0.0002069	Paxs	489.35	Joback Method
dvisc	0.0000957	Paxs	535.52	Joback Method
dvisc	0.0000500	Paxs	581.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3236484&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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