cyclohexapentylose

Other names:	.alpha.-cyclodextrin
	cyclohexaamylose
	«alpha»-Cyclodextrin
Inchi:	InChI=1S/C36H60O30/c37-1-7-25-13(43)19(49)31(55-7)62-26-8(2-38)57-33(21(51)15(26
InchiKey:	HFHDHCJBZVLPGP-OQDZSFIYSA-N
Formula:	C36H60O30
SMILES:	OCC1OC2OC3C(CO)OC(OC4C(CO)OC(OC5C(CO)OC(OC6C(CO)OC(OC7C(CO)OC(O
Mol. weight [g/mol]:	972.84
CAS:	10016-20-3

Physical Properties

Property code	Value	Unit	Source
gf	-3250.14	kJ/mol	Joback Method
hf	-5198.09	kJ/mol	Joback Method
hfus	225.81	kJ/mol	Joback Method
hvap	445.97	kJ/mol	Joback Method
log10ws	3.73		Crippen Method
logp	-13.055		Crippen Method
mcvol	618.180	ml/mol	McGowan Method
pc	1665.97	kPa	Joback Method
tb	3035.16	K	Joback Method
tf	1863.22	K	Joback Method
vc	2.154	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	-4554.46	J/mol×K	3035.16	Joback Method
cpg	1181.50	J/mol×K	332.68	Joback Method
cpg	2567.48	J/mol×K	1233.51	Joback Method
cpg	790.29	J/mol×K	2134.33	Joback Method

cps	1282.60	J/mol×K	328.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	1335.30	J/mol×K	338.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	1305.30	J/mol×K	333.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	1364.60	J/mol×K	343.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	1401.60	J/mol×K	348.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	1442.60	J/mol×K	353.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	1502.70	J/mol×K	358.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	1074.60	J/mol×K	288.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	1113.20	J/mol×K	293.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides

cps	1150.00	J/mol×K	298.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	1164.10	J/mol×K	303.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	1201.50	J/mol×K	308.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	1212.60	J/mol×K	313.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	1230.20	J/mol×K	318.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	1259.30	J/mol×K	323.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	1153.00	J/mol×K	298.15	NIST Webbook
dvisc	0.0000000	Pa×s	3035.16	Joback Method
dvisc	0.0000000	Pa×s	2839.84	Joback Method
dvisc	0.0000000	Pa×s	2644.51	Joback Method
dvisc	0.0000000	Pa×s	2449.19	Joback Method
dvisc	0.0000000	Pa×s	2253.87	Joback Method
dvisc	0.0000000	Pa×s	2058.54	Joback Method
dvisc	0.0000000	Pa×s	1863.22	Joback Method

Sources

A volumetric approach: Interactions of some local anesthetical drugs with alpha-cyclodextrin in aqueous solutions at 298.15 K:	https://www.doi.org/10.1016/j.jct.2016.12.023
Thermodynamic studies of drug - alpha-cyclodextrin interactions in water at 298.15 K: Procaine hydrochloride/lidocaine hydrochloride/tetracaine hydrochloride/ropivacaine hydrochloride + alpha-cyclodextrin + H2O systems:	https://www.doi.org/10.1016/j.jct.2013.09.003
Measurement and correlation of solubilities of the poorlywater-soluble pharmaceutical compound etodolac by addition of co-solvents:	https://www.doi.org/10.1016/j.fluid.2013.05.025
alpha-Cyclodextrin + Water binary system. New data on dehydration of alpha-cyclodextrin hexahydrate:	https://www.doi.org/10.1016/j.jct.2016.06.008
Effect of presence of alpha-cyclodextrin and beta-cyclodextrin on solution behavior of sulfathiazole at different temperatures: Thermodynamic and spectroscopic studies:	https://www.doi.org/10.1016/j.jct.2017.12.017
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Binary Mutual Diffusion Coefficients of Aqueous Solutions of r-Cyclodextrin, 2-Hydroxypropyl-r-cyclodextrin, and 2-Hydroxypropyl-a-cyclodextrin at Temperatures from (298.15 to 312.15) K:	https://www.doi.org/10.1021/je060474z
Limiting diffusion coefficients of sodium octanoate and octanoic acid in aqueous solutions without and with .alpha.-cyclodextrin:	https://www.doi.org/10.1016/j.jct.2015.11.013
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Activity Coefficient Studies in Ternary Aqueous Solutions at 298.15 K: H2O + r-Cyclodextrin + Potassium Acetate and H2O + 18-Crown-6 + Hydroquinone Systems:	https://www.doi.org/10.1021/je800307g
Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides:	https://www.doi.org/10.1016/j.jct.2008.08.007
Effect of different excipients on aqueous solubility of leflunomide: Thermodynamic study:	https://www.doi.org/10.1016/j.tca.2016.08.010
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10016203&Units=SI

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