Cycloheptanol

Other names: SUBEROL
Inchi: InChI=1S/C7H14O/c8-7-5-3-1-2-4-6-7/h7-8H,1-6H2
InchiKey: QCRFMSUKWRQZEM-UHFFFAOYSA-N
Formula: C7H14O
SMILES: OC1CCCCCC1
Mol. weight [g/mol]: 114.19
CAS: 502-41-0

Physical Properties

Property code	Value	Unit	Source
chl	-4429.20	kJ/mol	NIST Webbook
chl	-4362.00 ± 1.00	kJ/mol	NIST Webbook
gf	-116.41	kJ/mol	Joback Method
hf	-291.88	kJ/mol	Joback Method
hfus	7.71	kJ/mol	Joback Method
hvap	48.46	kJ/mol	Joback Method
log10ws	-0.88		Aqueous Solubility Prediction Method
log10ws	-0.88		Estimated Solubility Method
logp	1.701		Crippen Method
mcvol	104.500	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
rinpol	1028.00		NIST Webbook
rinpol	1022.00		NIST Webbook
rinpol	1040.20		NIST Webbook
ripol	1566.00		NIST Webbook
ripol	1547.00		NIST Webbook
ripol	1566.00		NIST Webbook
ripol	1566.00		NIST Webbook
sl	241.64	J/mol×K	NIST Webbook
tb	458.20	K	NIST Webbook
tc	675.73	K	Joback Method
tf	233.33	K	Joback Method
tt	280.30 ± 0.02	K	NIST Webbook
vc	0.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.00	J/mol×K	475.56	Joback Method
cpg	258.94	J/mol×K	542.28	Joback Method
cpg	272.33	J/mol×K	575.64	Joback Method
cpg	285.01	J/mol×K	609.00	Joback Method
cpg	297.01	J/mol×K	642.37	Joback Method
cpg	308.33	J/mol×K	675.73	Joback Method
cpg	244.83	J/mol×K	508.92	Joback Method
cpl	250.22	J/mol×K	298.15	NIST Webbook
cpl	244.30	J/mol×K	298.00	NIST Webbook
cps	199.80	J/mol×K	266.00	Heat capacities of selected cycloalcohols
cps	204.00	J/mol×K	270.00	Heat capacities of selected cycloalcohols
cps	199.80	J/mol×K	266.00	Heat capacities of selected cycloalcohols
cps	205.20	J/mol×K	271.34	Heat capacities of selected cycloalcohols
cps	205.40	J/mol×K	271.43	Heat capacities of selected cycloalcohols
cps	201.70	J/mol×K	268.00	Heat capacities of selected cycloalcohols
cps	201.80	J/mol×K	268.00	Heat capacities of selected cycloalcohols
cps	198.10	J/mol×K	264.00	Heat capacities of selected cycloalcohols
cps	198.00	J/mol×K	264.00	Heat capacities of selected cycloalcohols
cps	196.50	J/mol×K	262.00	Heat capacities of selected cycloalcohols
cps	196.40	J/mol×K	262.00	Heat capacities of selected cycloalcohols
cps	195.40	J/mol×K	260.73	Heat capacities of selected cycloalcohols

cps	204.00	J/mol×K	270.00	Heat capacities of selected cycloalcohols
cps	195.30	J/mol×K	260.59	Heat capacities of selected cycloalcohols
dvisc	0.0183260	Pa×s	273.70	Joback Method
dvisc	0.1241815	Pa×s	233.33	Joback Method
dvisc	0.0001677	Pa×s	475.56	Joback Method
dvisc	0.0003026	Pa×s	435.19	Joback Method
dvisc	0.0006163	Pa×s	394.82	Joback Method
dvisc	0.0014757	Pa×s	354.44	Joback Method
dvisc	0.0044230	Pa×s	314.07	Joback Method
hfust	0.88	kJ/mol	258.40	NIST Webbook
hfust	2.93	kJ/mol	172.20	NIST Webbook
hfust	1.60	kJ/mol	280.30	NIST Webbook
hfust	1.60	kJ/mol	280.30	NIST Webbook
hfust	1.51	kJ/mol	278.30	NIST Webbook
hfust	0.55	kJ/mol	227.30	NIST Webbook
hvapt	67.40	kJ/mol	302.50	NIST Webbook
hvapt	64.70	kJ/mol	303.50	NIST Webbook
pvap	0.12	kPa	315.14	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.16	kPa	319.51	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	7.10e-03	kPa	284.35	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

pvap	7.50e-03	kPa	284.67	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	0.01	kPa	288.22	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	0.02	kPa	292.50	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	0.18	kPa	320.88	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	0.02	kPa	293.73	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	

pvap	0.02	kPa	293.86	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	0.03	kPa	298.23	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	0.03	kPa	298.28	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	0.03	kPa	298.44	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	0.04	kPa	303.37	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	

pvap	0.06	kPa	307.00	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.07	kPa	308.15	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.08	kPa	310.11	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.02	kPa	293.72	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
sfust	16.98	J/mol×K	172.20	NIST Webbook
sfust	2.44	J/mol×K	227.30	NIST Webbook
sfust	5.72	J/mol×K	280.30	NIST Webbook
sfust	3.39	J/mol×K	258.40	NIST Webbook
srf	0.03	N/m	293.15	Surface Tensions of Dilute Solutions of Cycloheptanol in Ethylene Glycol
srf	0.03	N/m	313.15	Surface Tensions of Dilute Solutions of Cycloheptanol in Ethylene Glycol

srf	0.02	N/m	323.15	Surface Tensions of Dilute Solutions of Cycloheptanol in Ethylene Glycol
srf	0.03	N/m	298.15	Surface Tensions of Dilute Solutions of Cycloheptanol in Ethylene Glycol
srf	0.03	N/m	303.15	Surface Tensions of Dilute Solutions of Cycloheptanol in Ethylene Glycol
srf	0.03	N/m	308.15	Surface Tensions of Dilute Solutions of Cycloheptanol in Ethylene Glycol
srf	0.03	N/m	318.15	Surface Tensions of Dilute Solutions of Cycloheptanol in Ethylene Glycol

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	-2.66915e+01
Coeff. B	-5.85520e+03
Coeff. C	7.60167e+00
Coeff. D	-6.45886e-06
Temperature range (K), min.	284.15
Temperature range (K), max.	323.15

Sources

Heat capacities of selected cycloalcohols:	https://www.doi.org/10.1016/j.tca.2014.10.002
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Surface Tensions of Dilute Solutions of Cycloheptanol in Ethylene Glycol:	https://www.doi.org/10.1021/je050055m
KDB:	https://www.cheric.org/files/research/kdb/mol/mol900.mol

Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols:	https://www.doi.org/10.1021/acs.jced.6b00576
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C502410&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=900
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume