ARTEMISININ

Other names: 3,12-Epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6,9-trimethyl-, (3R,5aS,6R,8aS,9R,12S,12aR)-
Artemesinin

Inchi: InChI=1S/C15H22O5/c1-8-4-5-11-9(2)12(16)17-13-15(11)10(8)6-7-14(3,18-13)19-20-15/

InchiKey: BLUAFEHZUWYNDE-DFFGHCKCSA-N

Formula: C15H22O5

SMILES: CC1CCC2C(C)C(=O)OC3OC4(C)CCC1C32OO4

Mol. weight [g/mol]: 282.33

CAS: 63968-64-9

Physical Properties

Property code	Value	Unit	Source
gf	-231.16	kJ/mol	Joback Method
hf	-782.61	kJ/mol	Joback Method
hfus	24.30	kJ/mol	Solubility of Artemisinin in Different Single and Binary Solvent Mixtures Between (284.15 and 323.15) K and NRTL Interaction Parameters
hvap	68.38	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.395		Crippen Method
mcvol	203.820	ml/mol	McGowan Method
pc	2384.19	kPa	Joback Method
rinpol	1919.00		NIST Webbook
rinpol	1919.00		NIST Webbook
tb	748.73	K	Joback Method
tc	1001.60	K	Joback Method
tf	421.43	K	Standard Molar Enthalpies of Formation and Thermal Stabilities of Artemisinin and Its Two Derivatives: Artemether and Artesunate
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	832.02	J/mol×K	1001.60	Joback Method
cpg	808.51	J/mol×K	959.46	Joback Method
cpg	785.84	J/mol×K	917.31	Joback Method
cpg	763.67	J/mol×K	875.17	Joback Method
cpg	741.62	J/mol×K	833.02	Joback Method
cpg	719.34	J/mol×K	790.88	Joback Method
cpg	696.45	J/mol×K	748.73	Joback Method
cps	106.29	J/mol×K	80.88	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	133.57	J/mol×K	104.91	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	137.36	J/mol×K	107.91	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	141.04	J/mol×K	110.85	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	144.58	J/mol×K	113.72	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	147.72	J/mol×K	116.65	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	151.40	J/mol×K	119.63	Low temperature molar heat capacities and thermal stability of crystalline artemisinin

cps	154.67	J/mol×K	122.57	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	158.04	J/mol×K	125.44	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	161.18	J/mol×K	128.38	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	164.32	J/mol×K	131.37	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	167.29	J/mol×K	134.31	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	170.20	J/mol×K	137.21	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	173.58	J/mol×K	140.06	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	175.98	J/mol×K	142.85	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	178.74	J/mol×K	145.70	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	181.39	J/mol×K	148.61	Low temperature molar heat capacities and thermal stability of crystalline artemisinin

cps	184.15	J/mol×K	151.48	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	188.26	J/mol×K	154.31	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	189.51	J/mol×K	157.09	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	190.78	J/mol×K	159.85	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	193.14	J/mol×K	162.66	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	194.65	J/mol×K	165.54	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	196.91	J/mol×K	168.38	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	197.84	J/mol×K	171.20	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	199.03	J/mol×K	173.98	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	201.03	J/mol×K	176.74	Low temperature molar heat capacities and thermal stability of crystalline artemisinin

cps	203.22	J/mol×K	179.47	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	204.81	J/mol×K	182.17	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	207.17	J/mol×K	184.93	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	209.02	J/mol×K	187.75	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	210.20	J/mol×K	190.54	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	211.69	J/mol×K	193.30	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	214.53	J/mol×K	196.04	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	218.09	J/mol×K	198.78	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	234.61	J/mol×K	201.49	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	248.75	J/mol×K	204.35	Low temperature molar heat capacities and thermal stability of crystalline artemisinin

cps	254.52	J/mol×K	207.26	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	259.16	J/mol×K	210.15	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	263.67	J/mol×K	213.03	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	268.33	J/mol×K	215.98	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	272.61	J/mol×K	218.98	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	277.47	J/mol×K	221.97	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	283.14	J/mol×K	224.93	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	300.11	J/mol×K	227.86	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	305.21	J/mol×K	230.90	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	304.08	J/mol×K	234.15	Low temperature molar heat capacities and thermal stability of crystalline artemisinin

cps	300.49	J/mol×K	237.20	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	312.96	J/mol×K	240.20	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	303.71	J/mol×K	243.25	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	290.19	J/mol×K	246.20	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	291.35	J/mol×K	249.15	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	292.72	J/mol×K	252.08	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	294.78	J/mol×K	254.99	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	295.87	J/mol×K	257.88	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	297.43	J/mol×K	260.75	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	299.57	J/mol×K	263.60	Low temperature molar heat capacities and thermal stability of crystalline artemisinin

cps	301.66	J/mol×K	266.43	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	304.16	J/mol×K	269.30	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	307.87	J/mol×K	272.21	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	309.22	J/mol×K	275.11	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	312.58	J/mol×K	278.48	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	315.57	J/mol×K	282.32	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	318.40	J/mol×K	286.12	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	323.79	J/mol×K	289.88	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	327.62	J/mol×K	293.71	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	331.62	J/mol×K	297.59	Low temperature molar heat capacities and thermal stability of crystalline artemisinin

cps	336.33	J/mol×K	301.45	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	339.95	J/mol×K	305.28	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	344.57	J/mol×K	309.08	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	351.73	J/mol×K	312.86	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	334.75	J/mol×K	316.64	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	337.71	J/mol×K	320.44	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	338.79	J/mol×K	324.16	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	344.42	J/mol×K	327.84	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	356.39	J/mol×K	331.58	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	360.69	J/mol×K	335.37	Low temperature molar heat capacities and thermal stability of crystalline artemisinin

cps	368.06	J/mol×K	339.11	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	376.18	J/mol×K	342.41	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	376.26	J/mol×K	345.26	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	129.96	J/mol×K	101.96	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	394.39	J/mol×K	350.96	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	397.54	J/mol×K	353.85	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	403.86	J/mol×K	356.81	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	413.08	J/mol×K	359.88	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	429.50	J/mol×K	363.03	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	126.22	J/mol×K	99.06	Low temperature molar heat capacities and thermal stability of crystalline artemisinin

cps	122.29	J/mol×K	96.08	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	118.77	J/mol×K	93.15	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	115.11	J/mol×K	90.28	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	111.29	J/mol×K	87.31	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	107.40	J/mol×K	84.39	Low temperature molar heat capacities and thermal stability of crystalline artemisinin
cps	388.36	J/mol×K	348.11	Low temperature molar heat capacities and thermal stability of crystalline artemisinin

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of Artemisinin in Different Single and Binary Solvent Mixtures between (284.15 and 328.15) K and NRTL Interaction Parameters:	https://www.doi.org/10.1021/je100125x
Standard Molar Enthalpies of Formation and Thermal Stabilities of Artemisinin and Its Two Derivatives: Artemether and Artesunate:	https://www.doi.org/10.1021/je7000039
Solubility of Artemisinin in Ethanol + Water from (278.2 to 343.2) K:	https://www.doi.org/10.1021/je0603426
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63968649&Units=SI
Measurement and correlation of solubility of artemisinin in supercritical carbon dioxide:	https://www.doi.org/10.1016/j.fluid.2009.05.018
Low temperature molar heat capacities and thermal stability of crystalline artemisinin:	https://www.doi.org/10.1016/j.tca.2007.04.007
Solubility of Artemisinin in Supercritical Carbon Dioxide: Experimental Determination and Correlation of Artemisinin s Solubility in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je025575l
Solubility of Artemisinin in Seven Different Pure Solvents from (283.15 to 323.15) K:	https://www.doi.org/10.1021/je060015y
	https://www.doi.org/10.1021/je800515w

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume