

Cyanocobalamin

Other names:	vitamin B12
Inchi:	InChI=1S/C62H90N13O14P.CN.Co/c1-29-20-39-40(21-30(29)2)75(28-70-39)57-52(84)53
InchiKey:	RMRCNWBMXRMIRW-UHFFFAOYSA-L
Formula:	C63H88CoN14O14P
SMILES:	CC1=C2N=C(C=C3N=C(C(C)=C4NC(C)(C5N=C1C(C)(CCC(O)=NCC(C)OP(=O)(O)OC1
Mol. weight [g/mol]:	1355.37
CAS:	68-19-9

Physical Properties

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	16.34	J/mol×K	10.04	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	17.75	J/mol×K	10.42	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	20.67	J/mol×K	11.04	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	23.28	J/mol×K	11.60	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	26.23	J/mol×K	12.21	Low-temperature heat capacity and thermodynamic functions of vitamin B12

cps	29.45	J/mol×K	12.83	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	32.91	J/mol×K	13.46	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	36.48	J/mol×K	14.11	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	40.46	J/mol×K	14.75	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	44.40	J/mol×K	15.40	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	48.53	J/mol×K	16.07	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	52.68	J/mol×K	16.74	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	56.79	J/mol×K	17.42	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	61.22	J/mol×K	18.11	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	65.76	J/mol×K	18.81	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	70.36	J/mol×K	19.51	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	75.13	J/mol×K	20.22	Low-temperature heat capacity and thermodynamic functions of vitamin B12

cps	84.87	J/mol×K	21.61	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	99.82	J/mol×K	23.71	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	115.30	J/mol×K	25.87	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	131.90	J/mol×K	28.07	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	149.10	J/mol×K	30.31	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	166.20	J/mol×K	32.58	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	183.40	J/mol×K	34.87	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	201.20	J/mol×K	37.22	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	219.00	J/mol×K	39.58	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	237.30	J/mol×K	41.96	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	255.00	J/mol×K	44.36	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	272.20	J/mol×K	46.78	Low-temperature heat capacity and thermodynamic functions of vitamin B12

cps	289.00	J/mol×K	49.21	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	306.60	J/mol×K	51.65	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	323.60	J/mol×K	54.11	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	340.40	J/mol×K	56.59	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	357.90	J/mol×K	59.07	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	374.80	J/mol×K	61.56	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	392.40	J/mol×K	64.06	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	410.30	J/mol×K	66.57	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	427.90	J/mol×K	69.08	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	445.20	J/mol×K	71.59	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	461.60	J/mol×K	74.09	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	477.80	J/mol×K	76.59	Low-temperature heat capacity and thermodynamic functions of vitamin B12

cps	493.20	J/mol×K	79.11	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	508.50	J/mol×K	81.63	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	523.60	J/mol×K	84.15	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	540.30	J/mol×K	86.69	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	556.20	J/mol×K	89.22	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	571.80	J/mol×K	91.77	Low-temperature heat capacity and thermodynamic functions of vitamin B12
cps	587.60	J/mol×K	94.32	Low-temperature heat capacity and thermodynamic functions of vitamin B12

Sources

Low-temperature heat capacity and thermodynamic functions of vitamin B12
NIST Webbook:

<https://www.doi.org/10.1016/j.tca.2014.02.025>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C68199&Units=SI>

Legend

cps: Solid phase heat capacity

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