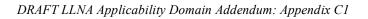


March 2009

APPENDIX C1

Physico-Chemical Properties and Chemical Classes of Metals Analyzed in the Applicability Domain of the LLNA



March 2009

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Physico-Chemical Properties – Metals (Sorted Alphabetically)

Substance Name	Synonyms	CASRN	Molecular Weight (g/mol)	Log Kow ¹	Physical Form	Chemical Class ²	Structure ³
Aluminum chloride	Aluminum chloride, anhydrous	7446-70-0	NA	NA	Solid	Inorganic Chemicals, Aluminum Compounds; Inorganic Chemicals, Chlorine Compounds	CI—AI
Ammonium tetrachloroplatinate ⁵	Ammonium platinous chloride, Ammonium chloroplatinate	13820-41-2	372.97	0.47	Solid	Inorganic Chemicals, Platinum Compounds	CIT NH ₄ -CI—Pt ² +-CIT CIT NH ₄
Beryllium sulfate	Beryllium sulfate tetrahydrate	7787-56-6	177.14	NA	Solid	Inorganic Chemicals; Metals; Salts	H ₂ O H ₂ O H ₂ O H ₂ O H ₂ O
Cobalt chloride	Cobaltous chloride	7646-79-9	129.84	0.85	Solid	Inorganic Chemicals; Metals; Salts	[CI ⁻] ^{ht} [Co ²⁺]
Cobalt (II) salts	NA	NA	NA	NA	Solid	Inorganic Chemicals; Metals; Salts	NA

Substance Name	Synonyms	CASRN	Molecular Weight (g/mol)	Log Kow ¹	Physical Form	Chemical Class ²	Structure ³
Cobalt sulfate	Cobaltous sulfate	10124-43-3	154.99	0.63	Solid	Inorganic Chemicals; Metals; Salts	o = ∞ - o - co²+
Copper chloride	Cuprous chloride	7758-89-6	98.99	-0.26	NA	Inorganic Chemicals; Metals; Salts	Cu—CI
Gold chloride	Gold tetrachloride	16903-35-8	339.79	0.16	Solid	Inorganic Chemicals, Gold Compounds; Salts	CI
Lead acetate	Acetic acid, lead salt	15347-57-6	325.29	-0.08	Solid	Inorganic Chemicals; Metals; Salts	O- PbH ₂ ²⁺ -O- CH ₃
Manganese chloride	Manganese chloride, anhydrous	7773-01-5	125.84	0.85	Solid	Inorganic Chemicals, Manganese Compounds; Salts	CI CI

Substance Name	Synonyms	CASRN	Molecular Weight (g/mol)	Log Kow ¹	Physical Form	Chemical Class ²	Structure ³
Mercuric chloride	Mercuric (II) chloride	7487-94-7	271.5	0.15	Solid	Inorganic Chemicals, Mercury Compounds; Salts	CI-HgCI
Nickel chloride	Nickelous chloride	7718-54-9	129.6	0.05	Solid	Inorganic Chemicals; Metals; Salts	cI—Ni
Nickel (II) salts	NA	NA	NA	NA	Solid	Inorganic Chemicals; Metals; Salts	NA
Nickel sulfate	Nickel (II) sulfate	7786-81-4	154.76	-0.17	Solid	Inorganic Chemicals; Metals; Salts	o = s − o- Ni ²⁺
Potassium dichromate	PDC	7778-50-9	294.18	-2.24	Solid	Inorganic Chemicals, Chromium Compounds; Inorganic Chemicals, Potassium Compounds	K* -0 - Cr 0 K*

Substance Name	Synonyms	CASRN	Molecular Weight (g/mol)	Log Kow ¹	Physical Form	Chemical Class ²	Structure ³
Tin chloride	NA	1344-13-14	260.52	NA	Solid	Inorganic Chemicals, Tin Compounds; Salts	CI ⁻ Sn ⁴⁺ CI ⁻
Zinc sulfate	Sulfuric acid, zinc salt; Zinc sulphate	7733-02-0	NA	NA	Solid	Inorganic Chemicals, Zinc Compounds; Salts	$0 = \begin{matrix} 0 \\ I \\ S - 0 \end{matrix}$ Zn^{2+}

Bold, italicized text represent the 11 metals reported in the original LLNA Evaluation Report (ICCVAM 1999).

Abbreviations: CASRN=Chemical Abstract Services Registry Number; g/mol=Grams per mole; Kow=Octanol-water partition coefficient; NA=Not available.

¹K_{ow} represents the octanol-water partition coefficient (expressed on log scale) obtained from the website: http://www.syrres.com/esc/est_kowdemo.htm.

²Chemical classifications based on the Medical Subject Headings classification for chemicals and drugs, as developed by the National Library of Medicine at: http://www.nlm.nih.gov/mesh/meshhome.html.

³Chemical structures, based on CASRN, were obtained from ChemID available at: http://chem.sis.nlm.nih.gov/chemidplus/chemidheavy.jsp.