

compound no	supplier	product no	lot no	purity	MW (g/mol)	name	signal word	notable hazards	hazard statements	precautionary statements	storage conditions	flash point	protection required	other info	mg for 100 mL of 1 uM	actual mg	mass uncertainty (mg)	actual concentration (mM)	concentration uncertainty (mM)	relative concentration uncertainty (%)	MW (g/mol) for HCl salt	corrected concentration for HCl salt without purity accounted for (mM)	corrected concentration uncertainties for HCl salt without accounting for purity (mM)	relative concentration uncertainty of HCl salt without accounting for purity (%)	smiles
C021	unknown	unknown		>95	192.9532	Cocurbit(7)ene hydrate		not a dangerous substance according to GHS						https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4343434/	116.23932	116.5	0.1	1.952	0.001	0.12%	1453.704	0.801	0.001	0.12%	
1	TCI	21215	80X1M-CQ	>92%	136.15	2-Xylenediamine	Danger	causes severe skin burns and eye damage		P201+P203-P305+P351+P338					12.015						209.12	0.000	#DIV/0!	#DIV/0!	Cl.C1NC1=CC=C(C=C1)
2	SIGMA-Aldrich	122020804	500070861	93.100%	87.08	2,2-Dimethyl-1-oxopiperidine	Danger	toxic by ingestion	H226-H302-H314	P201+P203-P305+P351+P338					8.716						123.62	0.000	#DIV/0!	#DIV/0!	Cl.CC(C)(C)CN
3	Alfa Aesar	L14157	H23R035	97%	117.19	6-Amino-1-hexanol	Warning	irritant, hygroscopic	H315-H319-H335	P201+P203-P305+P351+P338					11.719						153.65	0.000	#DIV/0!	#DIV/0!	C1NCCCCCO
4	AVOCADO		14212 C15536			Hexamethylenediamine	Danger	acute oral, dermal toxicity corrosive eye and skin							0						189.19	0.000	#DIV/0!	#DIV/0!	C1NCCCCCN
5	Alfa Aesar	L14058	823F15	88%	114.15	1,4-Bis(2-aminoethyl)benzene	Danger	causes severe skin burns and eye damage	H314	P201+P203-P305+P351+P338	store 2-8 °C, under water inert gas, sealed in CO2	70 °C			11.416						187.11	0.000	#DIV/0!	#DIV/0!	Cl.C1NCC(CCN)C1
6	Alfa Aesar	825070	121W014	97%?	151.03	trans-4-Aminocyclohexanol	Warning	causes skin irritation; causes severe eye irritation; may cause respiratory irritation	H315-H319-H335	P201+P305+P351+P338					15.163	16.3	0.1	1.076	0.007	0.62%	151.63	1.075	0.007	0.62%	C1NCCC(CO)C1
7	TCI	25604	2761-FLN	>99.0%	96.08	Cyclohexylamine	Danger	flammable liquid; highly toxic by ingestion; toxic by skin absorption; irritant, corrosive	H226-H302+H311-H314-H361-H402	P201+P203-P305+P351+P338		27 °C			9.818						135.64	0.000	#DIV/0!	#DIV/0!	C1NCCC(C1)N
8	Alfa Aesar	L51099	1013428	97%	113.2	Cyclohexylamine	Warning	combustible liquid; irritant	H226-H315-H335	P201		47 °C			11.32	12.1	0.1	1.069	0.009	0.83%	149.66	0.808	0.007	0.83%	C1NCCCCC1
9	Alfa Aesar	82681	1012028	99%	127.08	2-cyclohexylamine	Danger	combustible liquid; corrosive	H227-H314	P201+P203-P305+P351+P338		82 °C		white rubber gloves (min. 0.15 mm thickness, breakthrough time >30 min), tightly fitting safety goggles, chemical-resistant gloves	13.325						163.69	0.000	#DIV/0!	#DIV/0!	C1NCCCCC1
10	SIGMA-Aldrich	A55209		88%	125.2	1-(2-Aminomethyl)piperazine	Danger	combustible liquid; toxic by skin absorption; skin sensitizer; corrosive; extremely destructive to tissues of mucous membranes and upper respiratory tract; causes skin and eye burns	H227-H302+H311-H314-H373-H412	P201+P203-P305+P351+P338		82 °C			12.92						238.59	0.000	#DIV/0!	#DIV/0!	C1O.C1NCCN(C1)
11	SIGMA-Aldrich	179504	BOBB0243V	99%	111.18	exo-2-Aminonortornane	Warning	irritant	H226-H315-H319-H335	P201+P305+P351+P338		35 °C			11.118	11.3	0.1	1.016	0.009	0.89%	147.65	0.765	0.007	0.89%	C1C1(C)C2CCC(C2)
12	SIGMA-Aldrich	380039	1356334V			1,7,7-TRIMETHYLBICYCLO [2.2.1]HEPTAN-2-AMINE HYDROCHLORIDE	Warning	no known hazards, may be an irritant							0						189.73	0.000	#DIV/0!	#DIV/0!	Cl.C1(C)C2CCC(C2)
13	TCI	N0778	UQQLM-HM	>98%	173.68	Hydrochloride	Warning	skin and eye irritation	H315-H319-H335	P201+P305+P351+P338					17.368	18.1	0.1	1.042	0.005	0.56%	173.68	1.042	0.005	0.56%	C1NCCC(CCN)C1
14	Ark Pharm, Inc.	AK-44067	W20110324-012	>95%	187.248	3-Amino-1-adamantanol	Warning	harmful if swallowed; irritating to eyes, respiratory system, and skin	H302-H315-H319-H335	P201+P305+P351+P338	store 2-4 °C				16.7248	17.8	0.1	1.064	0.005	0.57%	203.71	0.874	0.005	0.57%	C1NCCC(CCN)C1