Cohesive energies for four different crystals

The red numbers were calculated by Quantum Espresso (PBE). The blue numbers are calculated based upon the red ones (please verify).

Cohesive energy per formula unit (or per mole) = [total energy of the corresponding amount of free atoms]   minus   [total energy of one formula unit (or mole) of the crystalline material]

material	# atoms per primitive cell	total energy per primitive cell (Ry)	total energy for free atom (Ry)	Cohesive energy (eV/formula unit)	Cohesive energy (kcal/mol)	Cohesive energy per atom (eV)
fcc-Al	1	-39.50286953	-39.24353150	3.53	81.2	3.53
fcc-Ar	1	-95.08508031	-95.08302073	0.03	0.7	0.03
germanium	2	-631.07725832	-315.26436826	3.73	85.9	3.73
halite (NaCl)	2	-188.85100486	-79.21682375 (Cl) -109.17614089 (Na)	6.23	143.5	3.11