item	Ed(kcal/mol)	Ed(kJ/mol)	PubChem C	Adsorbate	Adsorbent	comment	reference
1	53	221,752	12958	DMMP	γ–Al2O3 powder		Bermudez, J. Phys. Chem. C 2009, 113, 1917–1930
2	57,5	240,58	12958	DMMP	γ–Al2O3 powder	Al20O30cluster	Bermudez, J. Phys. Chem. C 2007, 111, 3719–3728
3	51,5	215,476	7871	Sarin GB	γ–Al2O3 powder		Bermudez, J. Phys. Chem. C 2009, 113, 1917–1930
4	33,3	139,3272	2483	TCPO	γ–Al2O3 powder	Al20O30cluster	Bermudez, Surface Science 602 (2008) 1938–1947
5	49	205,016	7871	Sarin GB	γ–Al2O3 powder	Al20O30cluster	Bermudez, Surface Science 602 (2008) 1938–1947
6	57,2	239,3248	12958	DMMP	γ–Al2O3 powder	Al20O30cluster	Bermudez, Surface Science 602 (2008) 1938–1947
7	62,2	260,2448	69609	TMPO	γ–Al2O3 powder	Al20O30cluster	Bermudez, Surface Science 602 (2008) 1938–1947
8	33	138,072	2483	TCPO	γ–Al2O3 powder	Al8O12cluster	Bermudez, Surface Science 602 (2008) 1938–1947
9	51,5	215,476	7871	Sarin GB	γ–Al2O3 powder	Al8O12cluster	Bermudez, Surface Science 602 (2008) 1938–1947
10	53	221,752	12958	DMMP	γ–Al2O3 powder	Al8O12cluster	Bermudez, Surface Science 602 (2008) 1938–1947
11	51,6	215,8944	178033	VX	γ–Al2O3 powder	Al8O12cluster	Bermudez, J. Phys. Chem. C 2009, 113, 1917–1930
12	58,6	245,1824	69609	TMPO	γ–Al2O3 powder	Al8O12cluster	Bermudez, Surface Science 602 (2008) 1938–1947
13	24,7	103,3448	2483	TCPO	γ–Al2O3 powder	Al32O48cluster	Bermudez, Surface Science 602 (2008) 1938–1947
14	39,8	166,5232	7871	Sarin GB	γ–Al2O3 powder	Al32O48cluster	Bermudez, Surface Science 602 (2008) 1938–1947
15	41,4	173,2176	12958	DMMP	γ–Al2O3 powder	Al32O48cluster	Bermudez, Surface Science 602 (2008) 1938–1947
16	39,3	164,4312	178033	VX	γ–Al2O3 powder	Al32O48cluster	Bermudez, J. Phys. Chem. C 2009, 113, 1917–1930
17	51,2	214,2208	69609	TMPO	γ–Al2O3 powder	Al32O48cluster	Bermudez, Surface Science 602 (2008) 1938–1947
18	13,2	55,2288	7871	Sarin GB	calcium oxide	CI calculus	J. Phys. Chem. C 118, 40, 23042-23048
19	6,4	26,7776	7871	Sarin GB	graphane	DFT calculus	J. Phys. Chem. C 118, 40, 23042-23048
20	4,8	20,0832	7871	Sarin GB	graphene	DFT calculus	J. Phys. Chem. C 118, 40, 23042-23048
21	18,8	78,6592	7871	Sarin GB	CaO (calcium oxide	DFT calculus	J. Phys. Chem. C 118, 40, 23042-23048
22	21	87,864	12958	DMMP	TiO2	O=P	Surface Science 604 (2010) 706–712
23	42,5	177,82	12958	DMMP	TiO2	(001)(1x1) OH free	Bermudez, J. Phys. Chem. C 2011, 115, 6741–6747
24	58,4	244,3456	12958	DMMP	TiO2	(001)(4x1) OH free	Bermudez, J. Phys. Chem. C 2011, 115, 6741–6747
25	5,4	22,5936	8030	thiophene	TiO2	(001)(1x1) OH free	Bermudez, J. Phys. Chem. C 2011, 115, 6741–6747
26		0	7305	Soman GD			
27		0	64505	Cyclosarin GF			
28	11,875	49,685	10461	Sulfur Mustard HD	graphene	parallel SM molecu	L. Ebrahimi, A. Khanlarkhani, M. R. Vaezi, and M
28	6,125	25,627	10461	Sulfur Mustard HD	graphene	tiltted molecules to	L. Ebrahimi, A. Khanlarkhani, M. R. Vaezi, and M
29			5372798	Lewisite L			

30		6500	Tabun GA

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