



Database name:	SGTE Substances Database	Database version:	4.1
Database acronym:	SSUB4		
Database owner:	Scientific Group Thermodata Europe		
Database segment:	Substances and gaseous species		

Brief description

The SSUB4 Substances Database is a large thermochemical database containing over 5000 condensed compounds or gaseous species. SSUB4 is commercially available for use with TCC and TCW; also together with its subset SPOT4 for uses in the POT module.

Applications

Alloy design and engineering; Inorganic materials, gas phase chemistry.

The SSUB4 Substances Database by itself is particularly useful for:

- Tabulation of thermochemical data.
- Computations and tabulations of reactions and equilibrium constants.
- Computation of complex gas equilibria for multicomponent systems (with no solid solutions), such as CVD calculations, potential diagram calculations, high-temperature corrosion calculations, and so forth.

This database is also extremely useful whenever it is necessary to append additional data for some compound phases and gaseous phase to a system that has been defined with uses of some other specific solution and/or compound database for e.g. steels/Fe-alloys, Ti-/TiAl-/Al-/Mg-/Cu-/... based alloys, Ni-based superalloys, ionic oxides/sulfides/nitrides/...solutions, ceramics, slag, molten salts, solders, noble metal alloys, semi-/super-conductors, polymers, nuclear materials, minerals, aqueous solutions, and organic substances/solutions, among others, in various advanced applications of material systems and material processes.

Included Elements

Ac	Ag	Al	Am	Ar	As	At	Au	B	Ba	Be	Bi	Br	C	Ca	Cd	Ce
Cf	Cl	Cm	Co	Cr	Cs	Cu	Dy	Er	Es	Eu	F	Fe	Fm	Fr	Ga	Gd
Ge	H	He	Hf	Hg	Ho	I	In	Ir	K	Kr	La	Li	Lu	Mg	Mn	Mo
N	Na	Nb	Nd	Ne	Ni	Np	O	Os	P	Pa	Pb	Pd	Pm	Po	Pr	Pt
Pu	Ra	Rb	Re	Rh	Rn	Ru	S	Sb	Sc	Se	Si	Sm	Sn	Sr	Ta	Tb
Tc	Te	Th	Ti	Tl	Tm	U	V	W	Xe	Y	Yb	Zn	Zr	D	T	

Included Phases

More than 5000 condensed compounds or gaseous species are available in the SSUB4 database. The gaseous mixture phase is the only solution phase in the database, and it is treated as ideal (in both EOS and mixing behaviors) at all temperatures, pressures and compositions.

Assessed Systems

The SSUB4 Substances Database contains assessed thermochemical data for 5254 substances (2902 condensed compounds and 2356 gaseous species) within a chemical framework of 101 elements.

The data for each compound or species consist of:

- The enthalpy of formation at 298.15 K (relative to pure elements).
- The entropy at 298.15 K (from 3rd law integrations or estimations).
- The temperature dependence of the heat capacity at constant pressure from 298.15 K up to the gaseous state.

Limits

Critical calculations must always be verified by equilibrium experimental data; it is the user's responsibility to verify the calculations but Thermo-Calc Software is interested to know about any significant deviations in order to improve any future release.

Scientific Models & References

See the Thermo-Calc Software reference list available at: <http://www.thermocalc.com/Library.htm>