

## Si

Source of data: JANAF [DIAMOND\_A4, LIQUID]  
Saunders et al. [BCC\_A2, FCC\_A1, HCP\_A3]  
Kaufman [BCC\_A12, CUB\_A13]

## Data for Si in the form of G-HSER

## DIAMOND\_A4

-8162.609 + 137.236859 T - 22.8317533 T ln(T) - 1.912904E-3 T<sup>2</sup> - 0.003552E-6 T<sup>3</sup> + 176667 T<sup>-1</sup> (298.15 < T < 1687)  
-9457.642 + 167.281367 T - 27.196 T ln(T) - 4.2037E30 T<sup>9</sup> (1687 < T < 3600)

## LIQUID

42533.751 + 107.13742 T - 22.8317533 T ln(T) - 1.912904E-3 T<sup>2</sup> - 0.003552E-6 T<sup>3</sup> + 176667 T<sup>-1</sup> + 2.0931E-21 T<sup>7</sup> (298.15 < T < 1687)  
40370.523 + 137.722298 T - 27.196 T ln(T) (1687 < T < 3600)

## BCC\_A2

38837.391 + 114.736859 T - 22.8317533 T ln(T) - 1.912904E-3 T<sup>2</sup> - 0.003552E-6 T<sup>3</sup> + 176667 T<sup>-1</sup> (298.15 < T < 1687)  
37542.358 + 144.781367 T - 27.196 T ln(T) - 4.2037E30 T<sup>9</sup> (1687 < T < 3600)

## FCC\_A1

42837.391 + 115.436859 T - 22.8317533 T ln(T) - 1.912904E-3 T<sup>2</sup> - 0.003552E-6 T<sup>3</sup> + 176667 T<sup>-1</sup> (298.15 < T < 1687)  
41542.358 + 145.481367 T - 27.196 T ln(T) - 4.2037E30 T<sup>9</sup> (1687 < T < 3600)

## BCC\_A12

42045.391 + 116.859859 T - 22.8317533 T ln(T) - 1.912904E-3 T<sup>2</sup> - 0.003552E-6 T<sup>3</sup> + 176667 T<sup>-1</sup> (298.15 < T < 1687)  
40750.358 + 146.904367 T - 27.196 T ln(T) - 4.2037E30 T<sup>9</sup> (1687 < T < 3600)

## CUB\_A13

39116.391 + 116.859859 T - 22.8317533 T ln(T) - 1.912904E-3 T<sup>2</sup> - 0.003552E-6 T<sup>3</sup> + 176667 T<sup>-1</sup> (298.15 < T < 1687)  
37821.358 + 146.904367 T - 27.196 T ln(T) - 4.2037E30 T<sup>9</sup> (1687 < T < 3600)

## HCP\_A3

41037.391 + 116.436859 T - 22.8317533 T ln(T) - 1.912904E-3 T<sup>2</sup> - 0.003552E-6 T<sup>3</sup> + 176667 T<sup>-1</sup> (298.15 < T < 1687)  
39742.358 + 146.481367 T - 27.196 T ln(T) - 4.2037E30 T<sup>9</sup> (1687 < T < 3600)

## Data for Si relative to DIAMOND\_A4

## LIQUID

50696.36 - 30.099439 T + 2.0931E-21 T<sup>7</sup> (298.15 < T < 1687.00)  
49828.165 - 29.559068 T + 4.2037E30 T<sup>9</sup> (1687.00 < T < 3600.00)

FCC\_A1

51000 - 21.8 T

 $(298.15 < T < 3600.00)$ 

BCC\_A2

47000 - 22.5 T

 $(298.15 < T < 3600.00)$ 

BCC\_A12

50208 - 20.377 T

 $(298.15 < T < 3600.00)$ 

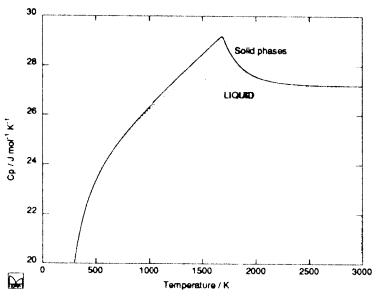
CUB\_A13

47279 - 20.377 T

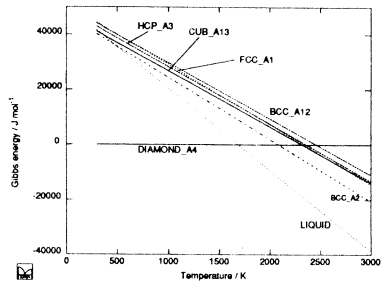
 $(298.15 < T < 3600.00)$ 

HCP\_A3

49200 - 20.8 T

 $(298.15 < T < 3600.00)$ 

Heat capacity of Si



Gibbs energy of phases of Si relative to DIAMOND\_A4