Heat of Reaction from Heats of Formation

Standard heat of reaction from the heats of formation and coefficients of up to three reactants and three products (Hess's law), per mole of reaction.

Method: Hess's law ΔH_r = Σν ΔH_f(products) − Σν ΔH_f(reactants)

Input parameters

Unit system: SI

Parameter	Value	Unit
Reactant 1: coefficient	1.0000	
Reactant 1: heat of formation	-74.870	kJ/mol
Reactant 2: coefficient	2.0000	
Reactant 2: heat of formation	0	kJ/mol
Reactant 3: coefficient	0	
Reactant 3: heat of formation	0	kJ/mol
Product 1: coefficient	1.0000	
Product 1: heat of formation	-393.51	kJ/mol
Product 2: coefficient	2.0000	
Product 2: heat of formation	-241.83	kJ/mol
Product 3: coefficient	0	
Product 3: heat of formation	0	kJ/mol

Calculated results

Parameter	Value	Unit
Heat of reaction (negative: exothermic)	-802.29	kJ/mol
Sum over products	-877.16	kJ/mol
Sum over reactants	-74.870	kJ/mol

Notes for this case

- Heats of formation of the right phase (gas or liquid water) at 25 °C from a property table; elements are zero.

Formula and method

$$\Delta H_r = \sum \nu_p \Delta H_{f,p} - \sum \nu_r \Delta H_{f,r}$$

Variables

ν_{r1}	Reactant 1: coefficient	-
$\Delta H_{f,r1}$	Reactant 1: heat of formation	J/mol
ν_{r2}	Reactant 2: coefficient	-
$\Delta H_{f,r2}$	Reactant 2: heat of formation	J/mol
ν_{r3}	Reactant 3: coefficient	-
$\Delta H_{f,r3}$	Reactant 3: heat of formation	J/mol
ν_{p1}	Product 1: coefficient	-
$\Delta H_{f,p1}$	Product 1: heat of formation	J/mol
ν_{p2}	Product 2: coefficient	-
$\Delta H_{f,p2}$	Product 2: heat of formation	J/mol
ν_{p3}	Product 3: coefficient	-

$\Delta H_{f,p3}$	Product 3: heat of formation	J/mol
ΔH_r	Heat of reaction (negative: exothermic)	J/mol
$\Sigma \nu \Delta H_f$	Sum over products	J/mol

Method and standards

Hess's law.

Assumptions and limits

- Standard state, 25 °C.
- The equation is not checked for balance: the species are entered only by their heats of formation, so balance the reaction yourself before entering the coefficients.

References

- Hess's law ΔH_r = Σν ΔH_f(products) − Σν ΔH_f(reactants)

Report details

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Release checks	3 reference cases of this calculator, computed independently, are checked on every release

Results are for engineering estimation. Verify critical designs against the referenced standards and your own data.

This calculator online

https://calc.firecad.com/chemical/mass-energy-balance/heat-of-reaction-formation

Open this case on calc.firecad.com →

Reopens the calculator with the inputs of this report.