

dinitrogen tetroxide

Other names: Dinitrogen tetroxide

Inchi: InChI=1S/N2O4/c3-1(4)2(5)6

InchiKey: WFPZPJSADLPSON-UHFFFAOYSA-N

Formula: N2O4

SMILES: O=[N+]([O-])[N+](=O)[O-]

Mol. weight [g/mol]: 92.01

CAS: 10544-72-6

Physical Properties

Property code	Value	Unit	Source
gf	20.22	kJ/mol	Joback Method
hf	-64.85	kJ/mol	Joback Method
hfus	18.48	kJ/mol	Joback Method
hvap	48.78	kJ/mol	Joback Method
ie	11.50 ± 0.10	eV	NIST Webbook
ie	11.60	eV	NIST Webbook
ie	11.00	eV	NIST Webbook
ie	11.40 ± 0.10	eV	NIST Webbook
ie	11.40 ± 0.10	eV	NIST Webbook
ie	10.80 ± 0.20	eV	NIST Webbook
ie	11.40 ± 0.10	eV	NIST Webbook
log10ws	-0.98		Crippen Method
logp	-0.545		Crippen Method
mcvol	45.700	ml/mol	McGowan Method
pc	7014.41	kPa	Joback Method
tb	503.08	K	Joback Method
tc	761.43	K	Joback Method
tf	376.98	K	Joback Method
vc	0.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	85.71	J/mol×K	503.08	Joback Method

cpg	89.43	J/mol×K	546.14	Joback Method
cpg	92.83	J/mol×K	589.20	Joback Method
cpg	95.93	J/mol×K	632.26	Joback Method
cpg	98.73	J/mol×K	675.31	Joback Method
cpg	101.25	J/mol×K	718.37	Joback Method
cpg	103.50	J/mol×K	761.43	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10544726&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Densities and Excess Molar Volumes of the Ternary System N₂O₄ + H₂O + HNO₃ at 258.2 K, 265.2 K, 273.2 K, and 281.2 K:	https://www.doi.org/10.1021/je101357s
Enthalpy Data for the N₂O₄ + H₂O + HNO₃ System at 258.2 K, 265.2 K, 273.2 K, and 281.2 K:	https://www.doi.org/10.1021/je800971f

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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