Nitrogen dioxide

Other names:	AZOTE
	NITROGEN PEROXIDE
	Nitrito
	Nitro
	Nitrogen dioxide (NO2)
	Nitrogen oxide
	Rcra waste number P078
	Stickstoffdioxid
	Stikstofdioxyde
	nitrogen oxide (NO2)
Inchi:	InChI=1S/NO2/c2-1-3
InchiKey:	JCXJVPUVTGWSNB-UHFFFAOYSA-N
Formula:	NO2
SMILES:	[O]N=O
Mol. weight [g/mol]:	46.01
CAS:	10102-44-0

Physical Properties

Property code	Value	Unit	Source
af	0.8340		KDB
affp	591.00	kJ/mol	NIST Webbook
basg	560.30	kJ/mol	NIST Webbook
dm	0.40	debye	KDB
ea	2.35 ± 0.10	eV	NIST Webbook
ea	3.10 ± 0.05	eV	NIST Webbook
ea	3.90 ± 0.20	eV	NIST Webbook
ea	2.07 ± 0.24	eV	NIST Webbook
ea	2.04	eV	NIST Webbook
ea	2.50 ± 0.10	eV	NIST Webbook
ea	2.50 ± 0.10	eV	NIST Webbook
ea	2.10	eV	NIST Webbook
ea	1.80 ± 0.20	eV	NIST Webbook
ea	2.60	eV	NIST Webbook
ea	1.80 ± 0.05	eV	NIST Webbook
ea	3.82	eV	NIST Webbook
ea	2.80 ± 0.05	eV	NIST Webbook
ea	2.11 ± 0.18	eV	NIST Webbook

ea	2.38 ± 0.06	eV	NIST Webbook
ea	2.27 ± 0.03	eV	NIST Webbook
ea	3.99	eV	NIST Webbook
ea	2.28 ± 0.10	eV	NIST Webbook
ea	2.40 ± 0.10	eV	NIST Webbook
ea	2.27 ± 0.01	eV	NIST Webbook
ea	2.30 ± 0.10	eV	NIST Webbook
ea	2.30 ± 0.15	eV	NIST Webbook
ea	2.36 ± 0.10	eV	NIST Webbook
ea	2.50 ± 0.05	eV	NIST Webbook
gf	52.00	kJ/mol	KDB
hf	33.87	kJ/mol	KDB
hfus	8.80	kJ/mol	Joback Method
hvap	32.04	kJ/mol	Joback Method
ie	9.59 ± 0.00	eV	NIST Webbook
ie	9.59 ± 0.00	eV	NIST Webbook
ie	11.23	eV	NIST Webbook
ie	10.40 ± 0.30	eV	NIST Webbook
ie	11.23	eV	NIST Webbook
ie	9.75 ± 0.01	eV	NIST Webbook
ie	9.62 ± 0.01	eV	NIST Webbook
ie	9.60 ± 0.03	eV	NIST Webbook
log10ws	-4.90		Crippen Method
logp	0.098		Crippen Method
mcvol	26.130	ml/mol	McGowan Method
pc	10100.00	kPa	KDB
tb	294.30	K	KDB
tb	295.08 ± 0.50	K	NIST Webbook
tc	431.00	K	KDB
tf	261.90	K	KDB
vc	0.168	m3/kmol	KDB
zc	0.4729330		KDB
zra	0.24		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	33.13	J/mol×K	350.54	Joback Method
cpg	35.27	J/mol×K	385.70	Joback Method
cpg	37.11	J/mol×K	420.87	Joback Method
cpg	38.66	J/mol×K	456.03	Joback Method

cpg	39.96	J/mol×K	491.20	Joback Method
cpg	41.04	J/mol×K	526.36	Joback Method
cpg	41.93	J/mol×K	561.53	Joback Method
rhol	1450.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.04197e+01
Coeff. B	-5.27208e+03
Coeff. C	3.95000e+01
Temperature range (K), min.	261.95
Temperature range (K), max.	431.35

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental study of high pressure phase equilibrium of (CO2 + NO2/N2O4) mixtures:	https://www.doi.org/10.1016/j.jct.2011.07.007
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1929
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10102440&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
dm:	Dipole Moment
ea:	Electron affinity

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
pvap:	Vapor pressure
rhol:	Liquid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter