ozone

Other names: TRIATOMIC OXYGEN
Inchi: InChI=1S/O3/c1-3-2
InchiKey: CBENFWSGALASAD-UHFFFAOYSA-N
Formula: O3
SMILES: O=[O+][O-]
Mol. weight [g/mol]: 48.00
CAS: 10028-15-6

Physical Properties

Property code	Value	Unit	Source
af	0.1947		KDB
affp	625.50	kJ/mol	NIST Webbook
basg	595.90	kJ/mol	NIST Webbook
dm	0.60	debye	KDB
ea	2.10 ± 0.00	eV	NIST Webbook
ea	2.14 ± 0.15	eV	NIST Webbook
ea	1.91 ± 0.14	eV	NIST Webbook
ea	1.82	eV	NIST Webbook
ea	1.96	eV	NIST Webbook
ea	2.10 ± 0.00	eV	NIST Webbook
gf	162.90	kJ/mol	KDB
hf	142.80	kJ/mol	KDB
ie	12.80 ± 0.05	eV	NIST Webbook
ie	12.67	eV	NIST Webbook
ie	12.56	eV	NIST Webbook
ie	12.44 ± 0.01	eV	NIST Webbook
ie	12.50 ± 0.10	eV	NIST Webbook
ie	12.53 ± 0.08	eV	NIST Webbook
ie	12.52 ± 0.00	eV	NIST Webbook
ie	12.73	eV	NIST Webbook
ie	12.43	eV	NIST Webbook
ie	12.89 ± 0.10	eV	NIST Webbook
ie	12.30 ± 0.10	eV	NIST Webbook
log10ws	-2.87		Crippen Method
logp	-1.122		Crippen Method
mcvol	24.170	ml/mol	McGowan Method
pc	5570.00	kPa	KDB

tb	161.80	K	KDB
tb	161.30 ± 0.50	K	NIST Webbook
tc	261.05 ± 1.00	K	NIST Webbook
tc	261.10	K	KDB
tc	261.15 ± 1.50	K	NIST Webbook
tf	80.00	K	KDB
tf	80.70 ± 0.50	K	NIST Webbook
vc	0.089	m3/kmol	KDB
zc	0.2283500		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
rhol	1356.00	kg/m3	161.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44711e+01
Coeff. B	-1.42440e+03
Coeff. C	-1.72800e+01
Temperature range (K), min.	80.15
Temperature range (K), max.	261.00

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1937

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10028156&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
dm:	Dipole Moment
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation 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