Carbon tetrabromide

Other names:	Bromid uhlicity
	CARBONTETRABROMIDE
	CBr4
	Carbon bromide
	Carbon bromide (CBr4)
	Methane tetrabromide
	Methane, tetrabromo-
	NSC 6179
	REFRIGERANT-10B4
	Tetrabromomethane
	UN 2516
Inchi:	InChI=1S/CBr4/c2-1(3,4)5
InchiKey:	HJUGFYREWKUQJT-UHFFFAOYSA-N
Formula:	CBr4
SMILES:	BrC(Br)(Br)Br
Mol. weight [g/mol]:	331.63
CAS:	558-13-4

Physical Properties

Property code	Value	Unit	Source
chs	-422.90 ± 3.30	kJ/mol	NIST Webbook
ea	2.06	eV	NIST Webbook
gf	17.66	kJ/mol	Joback Method
hf	83.90 ± 3.40	kJ/mol	NIST Webbook
hfs	29.40 ± 3.40	kJ/mol	NIST Webbook
hfus	12.07	kJ/mol	Joback Method
hsub	54.50 ± 0.70	kJ/mol	NIST Webbook
hvap	42.26	kJ/mol	Joback Method
ie	10.31 ± 0.02	eV	NIST Webbook
ie	10.31 ± 0.02	eV	NIST Webbook
ie	10.40	eV	NIST Webbook
ie	10.39	eV	NIST Webbook
ie	10.54	eV	NIST Webbook
ie	10.30 ± 0.20	eV	NIST Webbook
ie	10.80 ± 0.30	eV	NIST Webbook
log10ws	-3.14		Aqueous Solubility Prediction Method

log10ws	-3.14		Estimated Solubility Method
logp	3.177		Crippen Method
mcvol	94.950	ml/mol	McGowan Method
nfpah	%!d(float64=3)		KDB
nfpas	%!d(float64=1)		KDB
pc	9630.56	kPa	Joback Method
rinpol	1046.00		NIST Webbook
rinpol	1054.00		NIST Webbook
rinpol	1050.00		NIST Webbook
rinpol	1046.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1050.00		NIST Webbook
ripol	1677.81		NIST Webbook
ripol	1690.77		NIST Webbook
tb	483.69	K	Joback Method
tc	757.88	K	Joback Method
tf	367.60 ± 1.00	K	NIST Webbook
tf	363.25	K	Aqueous Solubility Prediction Method
tf	363.25	K	KDB
tf	365.00 ± 0.50	K	NIST Webbook
tf	364.05 ± 0.40	K	NIST Webbook
vc	0.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	106.98	J/mol×K	757.88	Joback Method
cpg	104.31	J/mol×K	529.39	Joback Method
cpg	102.29	J/mol×K	483.69	Joback Method
cpg	107.03	J/mol×K	712.18	Joback Method
cpg	106.91	J/mol×K	666.48	Joback Method
cpg	106.49	J/mol×K	620.78	Joback Method
cpg	105.66	J/mol×K	575.09	Joback Method
cpl	162.30	J/mol×K	373.00	NIST Webbook
cps	128.66	J/mol×K	300.60	NIST Webbook
cps	148.40	J/mol×K	298.00	NIST Webbook
cps	145.90	J/mol×K	298.15	NIST Webbook
dvisc	0.0006326	Pa×s	460.18	Joback Method
dvisc	0.0023917	Pa×s	342.65	Joback Method

dvisc	0.0009834	Pa×s	413.17	Joback Method
dvisc	0.0007794	Pa×s	436.68	Joback Method
dvisc	0.0005239	Pa×s	483.69	Joback Method
dvisc	0.0017121	Pa×s	366.16	Joback Method
dvisc	0.0012760	Pa×s	389.66	Joback Method
hfust	3.95	kJ/mol	363.20	NIST Webbook
hfust	3.95	kJ/mol	363.20	NIST Webbook
hfust	5.94	kJ/mol	320.00	NIST Webbook
hvapt	48.20	kJ/mol	416.00	NIST Webbook
hvapt	48.30	kJ/mol	419.00	NIST Webbook
sfust	10.88	J/mol×K	363.20	NIST Webbook
sfust	18.58	J/mol×K	320.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.72437e+01
Coeff. B	-5.84669e+03
Coeff. C	3.90000e-01
Temperature range (K), min.	344.42
Temperature range (K), max.	489.60

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.34543e+02
Coeff. B	-1.60253e+04
Coeff. C	-3.25119e+01
Coeff. D	1.98033e-05
Temperature range (K), min.	369.15
Temperature range (K), max.	463.15

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1504.mol
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C558134&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1504
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume