Buckminsterfullerene

Other names:	carbon (C60)
	follene-60
	footballene
	footballene (C60)
	icosahedral C60
	soccerballene
Inchi:	InChI=1S/C60/c1-2-5-6-3(1)8-12-10-4(1)9-11-7(2)17-21-13(5)23-24-14(6)22-18(8)28-20(
InchiKey:	XMWRBQBLMFGWIX-UHFFFAOYSA-N
Formula:	C60
SMILES:	c12c3c4c5c1c1c6c7c2c2c8c3c3c9c4c4c%10c5c5c1c1c6c6c%11c7c2c2c7c8c3c3c8c9c4
Mol. weight [g/mol]:	720.64
CAS:	99685-96-8

Physical Properties

Property code	Value	Unit	Source
basg	827.50	kJ/mol	NIST Webbook
chs	-25937.00 ± 16.00	kJ/mol	NIST Webbook
chs	-25889.00 ± 12.00	kJ/mol	NIST Webbook
chs	-25884.00 ± 13.00	kJ/mol	NIST Webbook
chs	-25890.80 ± 5.40	kJ/mol	NIST Webbook
chs	-26033.00 ± 14.00	kJ/mol	NIST Webbook
chs	25965.00 ± 12.00	kJ/mol	NIST Webbook
ea	2.68 ± 0.00	eV	NIST Webbook
ea	2.68 ± 0.01	eV	NIST Webbook
ea	2.65 ± 0.05	eV	NIST Webbook
ea	2.47 ± 0.01	eV	NIST Webbook
ea	2.67 ± 0.00	eV	NIST Webbook
ea	2.70 ± 0.20	eV	NIST Webbook
ea	1.62 ± 0.19	eV	NIST Webbook
ea	2.69 ± 0.01	eV	NIST Webbook
gf	3296.88	kJ/mol	Joback Method
hf	2854.09	kJ/mol	Joback Method
hfus	142.76	kJ/mol	Joback Method
hsub	228.70 ± 7.30	kJ/mol	NIST Webbook
hsub	234.00	kJ/mol	NIST Webbook
hsub	181.10 ± 2.60	kJ/mol	NIST Webbook
hsub	183.50 ± 1.00	kJ/mol	NIST Webbook

hsub	184.10 ± 3.10	kJ/mol	NIST Webbook
hsub	179.20 ± 3.50	kJ/mol	NIST Webbook
hsub	180.00 ± 2.00	kJ/mol	NIST Webbook
hsub	183.20 ± 3.50	kJ/mol	NIST Webbook
hsub	180.60 ± 1.50	kJ/mol	NIST Webbook
hsub	168.50 ± 1.20	kJ/mol	NIST Webbook
hsub	181.00 ± 2.00	kJ/mol	NIST Webbook
hvap	198.84	kJ/mol	Joback Method
ie	7.80	eV	NIST Webbook
ie	7.58 ± 0.03	eV	NIST Webbook
ie	7.61 ± 0.11	eV	NIST Webbook
ie	7.60 ± 0.10	eV	NIST Webbook
ie	7.61 ± 0.02	eV	NIST Webbook
ie	7.60 ± 0.20	eV	NIST Webbook
ie	7.54 ± 0.04	eV	NIST Webbook
ie	7.57 ± 0.01	eV	NIST Webbook
ie	7.60	eV	NIST Webbook
ie	8.10 ± 0.50	eV	NIST Webbook
ie	7.61	eV	NIST Webbook
ie	8.10 ± 0.50	eV	NIST Webbook
ie	7.60 ± 0.50	eV	NIST Webbook
log10ws	-36.31		Crippen Method
logp	17.730		Crippen Method
mcvol	390.600	ml/mol	McGowan Method
pc	1514.03	kPa	Joback Method
tb	2058.60	K	Joback Method
tc	3046.14	K	Joback Method
tf	2343.70	K	Joback Method
vc	1.938	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	45805.13	J/mol×K	2881.55	Joback Method
cpg	11897.55	J/mol×K	2058.60	Joback Method
cpg	16327.11	J/mol×K	2223.19	Joback Method
cpg	21818.31	J/mol×K	2387.78	Joback Method
cpg	28485.48	J/mol×K	2552.37	Joback Method
cpg	36442.98	J/mol×K	2716.96	Joback Method
cpg	56686.28	J/mol×K	3046.14	Joback Method
cps	556.46	J/mol×K	300.00	NIST Webbook

cps	536.90	J/mol×K	298.15	NIST Webbook
cps	550.00	J/mol×K	300.00	NIST Webbook
dvisc	3316437621269424640.0	Pa×s	2058.60	Joback Method
dvisc	8211061978777230336.0000000	Pa×s	2343.70	Joback Method
dvisc	7170803679794909184.0	Pa×s	2296.18	Joback Method
dvisc	6226586038619201536.0000000	Pa×s	2248.67	Joback Method
dvisc	5373840763900083200.0	Pa×s	2201.15	Joback Method
dvisc	4607835880423360000.0000000	Pa×s	2153.63	Joback Method
dvisc	3923698028174746112.0	Pa×s	2106.12	Joback Method
hsubt	138.00 ± 4.00	kJ/mol	550.00	NIST Webbook
hsubt	152.80 ± 0.10	kJ/mol	848.00	NIST Webbook
hsubt	175.20 ± 2.90	kJ/mol	860.00	NIST Webbook
hsubt	180.00 ± 10.00	kJ/mol	634.00	NIST Webbook
hsubt	158.00 ± 3.00	kJ/mol	700.00	NIST Webbook
hsubt	181.40 ± 2.30	kJ/mol	700.00	NIST Webbook
hsubt	158.60	kJ/mol	773.00	NIST Webbook
hsubt	159.00 ± 4.20	kJ/mol	773.00	NIST Webbook
hsubt	160.00 ± 4.00	kJ/mol	673.00	NIST Webbook
hsubt	176.00 ± 2.00	kJ/mol	727.00	NIST Webbook
hsubt	168.00 ± 5.40	kJ/mol	707.00	NIST Webbook
hsubt	167.80 ± 5.40	kJ/mol	720.00	NIST Webbook
hvapt	175.00	kJ/mol	945.00	Enthalpies of sublimation of fullerenes by thermogravimetry

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Pressure dependence of the solubility of light fullerenes in n-nonane:	https://www.doi.org/10.1016/j.jct.2017.05.017
Enthalpies of combustion and formation of fullerenes by micro-combustion calorimetry in a Calvet bomb:	https://www.doi.org/10.1016/j.tca.2005.06.029
Enthalpies of sublimation of fullerenes by thermogravimetry :	https://www.doi.org/10.1016/j.tca.2015.09.001
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C99685968&Units=SI
Mass Diffusion Coefficient and Soret Coefficient of o-Dichlorobenzene Solutions of PCBM and [60]Fullerene by the Soret Forced Rayleigh Scattering Method:	https://www.doi.org/10.1021/acs.jced.5b00609
Temperature Dependence of Solubility of Individual Light Fullerenes and Industrial Fullerene Mixture in 1-Chloronaphthalene and 1-Bromonaphthalene:	https://www.doi.org/10.1021/je900814w

Legend

basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas 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
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume