Benzofuran

Other names:	1-Oxindene
	2,3-Benzofuran
	Benzo[b]furan
	Benzofurfuran
	Coumarone
	Cumarone
	NCI-C56166
Inchi:	InChI=1S/C8H6O/c1-2-4-8-7(3-1)5-6-9-8/h1-6H
InchiKey:	IANQTJSKSUMEQM-UHFFFAOYSA-N
Formula:	C8H6O
SMILES:	c1ccc2occc2c1
Mol. weight [g/mol]:	118.13
CAS:	271-89-6

Physical Properties

Property code	Value	Unit	Source
chl	-3970.74 ± 0.58	kJ/mol	NIST Webbook
hf	13.60 ± 0.70	kJ/mol	NIST Webbook
hfl	-34.83 ± 0.68	kJ/mol	NIST Webbook
hvap	48.40	kJ/mol	NIST Webbook
hvap	48.40 ± 0.20	kJ/mol	NIST Webbook
ie	8.37 ± 0.01	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
ie	8.36 ± 0.05	eV	NIST Webbook
ie	8.42	eV	NIST Webbook
ie	8.29 ± 0.05	eV	NIST Webbook
ie	8.85 ± 0.05	eV	NIST Webbook
log10ws	-7.01		Crippen Method
logp	2.433		Crippen Method
mcvol	90.530	ml/mol	McGowan Method
rinpol	156.70		NIST Webbook
rinpol	153.80		NIST Webbook
rinpol	153.20		NIST Webbook
rinpol	173.42		NIST Webbook
rinpol	160.51		NIST Webbook
rinpol	156.70		NIST Webbook
rinpol	153.20		NIST Webbook

rinpol	1015.00		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	1005.80		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	996.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	996.00		NIST Webbook
ripol	1496.00		NIST Webbook
ripol	1521.00		NIST Webbook
ripol	1489.00		NIST Webbook
ripol	1488.00		NIST Webbook
ripol	1486.00		NIST Webbook
ripol	1496.00		NIST Webbook
sl	215.59	J/mol×K	NIST Webbook
tb	447.20	K	NIST Webbook
tb	447.15 ± 0.50	K	NIST Webbook
tb	442.15 ± 1.50	K	NIST Webbook
tb	444.15 ± 0.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpl	178.70	J/mol×K	298.15	NIST Webbook
hvapt	46.20	kJ/mol	363.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	335.50 ± 0.50	K	2.00	NIST Webbook
tbrp	440.30 ± 0.70	K	98.00	NIST Webbook
tbrp	371.30 ± 0.70	K	11.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45265e+01
Coeff. B	-3.88945e+03
Coeff. C	-5.46010e+01
Temperature range (K), min.	327.76
Temperature range (K), max.	476.68

Sources

Liquid-Liquid Equilibrium Measurements for Model Systems Related to Catalytic Fast Pyrolysis of Biomass:	https://www.doi.org/10.1021/acs.jced.6b00625
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C271896&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpl:	Liquid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation 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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure