

Benzofuran, 2,3-dihydro-

Other names:	Coumaran Dihydrobenzofuran Dihydrocoumarone Kumaran 2,3-Dihydrobenzofuran 2,3-Dihydrobenzofurane Coumaran (2,3-dihydrobenzofuran)
Inchi:	InChI=1S/C8H8O/c1-2-4-8-7(3-1)5-6-9-8/h1-4H,5-6H2
InchiKey:	HBEDSQVIWPRPAY-UHFFFAOYSA-N
Formula:	C8H8O
SMILES:	c1ccc2c(c1)CCO2
Mol. weight [g/mol]:	120.15
CAS:	496-16-2

Physical Properties

Property code	Value	Unit	Source
chl	-4191.62 ± 0.62	kJ/mol	NIST Webbook
gf	101.60	kJ/mol	Joback Method
hf	-46.50 ± 0.80	kJ/mol	NIST Webbook
hfl	-99.78 ± 0.72	kJ/mol	NIST Webbook
hfus	15.17	kJ/mol	Joback Method
hvap	53.30	kJ/mol	NIST Webbook
hvap	53.30 ± 0.06	kJ/mol	NIST Webbook
ie	7.65	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.02	eV	NIST Webbook
log10ws	-1.87		Crippen Method
logp	1.621		Crippen Method
mcvol	94.830	ml/mol	McGowan Method
pc	4351.13	kPa	Joback Method
rinpol	1224.00		NIST Webbook
rinpol	1226.00		NIST Webbook
rinpol	1191.00		NIST Webbook
rinpol	1237.00		NIST Webbook
rinpol	1207.00		NIST Webbook
rinpol	1187.00		NIST Webbook
rinpol	1223.00		NIST Webbook

rinpol	1237.00		NIST Webbook
rinpol	1216.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1211.00		NIST Webbook
rinpol	1219.00		NIST Webbook
rinpol	1188.00		NIST Webbook
rinpol	1224.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1187.00		NIST Webbook
rinpol	1226.00		NIST Webbook
rinpol	175.30		NIST Webbook
sl	226.43	J/mol×K	NIST Webbook
tb	461.70	K	NIST Webbook
tc	681.73	K	Joback Method
tf	250.89	K	NIST Webbook
vc	0.354	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.41	J/mol×K	452.46	Joback Method
cpg	250.67	J/mol×K	681.73	Joback Method
cpg	242.14	J/mol×K	643.52	Joback Method
cpg	232.90	J/mol×K	605.31	Joback Method
cpg	222.87	J/mol×K	567.10	Joback Method
cpg	211.99	J/mol×K	528.88	Joback Method
cpg	200.19	J/mol×K	490.67	Joback Method
cpl	188.64	J/mol×K	298.15	NIST Webbook
dvisc	0.0004412	Pa×s	452.46	Joback Method
dvisc	0.0005189	Pa×s	421.65	Joback Method
dvisc	0.0006262	Pa×s	390.84	Joback Method
dvisc	0.0007802	Pa×s	360.04	Joback Method
dvisc	0.0010130	Pa×s	329.23	Joback Method
dvisc	0.0013881	Pa×s	298.42	Joback Method
dvisc	0.0020452	Pa×s	267.61	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	357.20	K	2.30	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C496162&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
rinpol:	Non-polar retention indices
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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