

Benzocyclobuten-1(2H)-one

Other names:	Benzocyclobutenone Bicyclo(4.2.0)octa-1,3,5-trien-7-one
Inchi:	InChI=1S/C8H6O/c9-8-5-6-3-1-2-4-7(6)8/h1-4H,5H2
InchiKey:	XOGFXHMYHKGOGP-UHFFFAOYSA-N
Formula:	C8H6O
SMILES:	O=C1Cc2ccccc21
Mol. weight [g/mol]:	118.13
CAS:	3469-06-5

Physical Properties

Property code	Value	Unit	Source
gf	77.23	kJ/mol	Joback Method
hf	-21.79	kJ/mol	Joback Method
hfus	8.80	kJ/mol	Joback Method
hvap	40.64	kJ/mol	Joback Method
ie	8.99	eV	NIST Webbook
log10ws	-1.99		Crippen Method
logp	1.425		Crippen Method
mcvol	90.530	ml/mol	McGowan Method
pc	4462.28	kPa	Joback Method
tb	489.06	K	Joback Method
tc	729.56	K	Joback Method
tf	312.78	K	Joback Method
vc	0.348	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.99	J/molxK	489.06	Joback Method
cpg	194.32	J/molxK	529.14	Joback Method
cpg	204.85	J/molxK	569.23	Joback Method
cpg	214.63	J/molxK	609.31	Joback Method
cpg	223.71	J/molxK	649.39	Joback Method
cpg	232.14	J/molxK	689.48	Joback Method

cpg

239.97

J/mol×K

729.56

Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	344.50 ± 0.50	K	0.30	NIST Webbook

Sources

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=C3469065&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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
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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