Benzene, 1-cyclobuten-1-yl-

Other names:	1-Phenyl-1-cyclobutene
	1-Phenylcyclobutene
Inchi:	InChI=1S/C10H10/c1-2-5-9(6-3-1)10-7-4-8-10/h1-3,5-7H,4,8H2
InchiKey:	KMWHNPPKABDZMJ-UHFFFAOYSA-N
Formula:	C10H10
SMILES:	C1=C(c2ccccc2)CC1
Mol. weight [g/mol]:	130.19
CAS:	3365-26-2

Physical Properties

Property code	Value	Unit	Source
gf	222.42	kJ/mol	Joback Method
hf	120.09	kJ/mol	Joback Method
hfus	11.49	kJ/mol	Joback Method
hvap	41.48	kJ/mol	Joback Method
ie	8.24	eV	NIST Webbook
ie	8.20 ± 0.05	eV	NIST Webbook
ie	8.22	eV	NIST Webbook
log10ws	-3.03		Crippen Method
logp	2.864		Crippen Method
mcvol	112.840	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
tb	474.70	K	Joback Method
tc	709.77	K	Joback Method
tf	260.82	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.37	J/mol×K	474.70	Joback Method
cpg	240.59	J/mol×K	513.88	Joback Method
cpg	254.65	J/mol×K	553.06	Joback Method
cpg	267.64	J/mol×K	592.23	Joback Method

cpg	279.62	J/mol×K	631.41	Joback Method
cpg	290.67	J/mol×K	670.59	Joback Method
cpg	300.86	J/mol×K	709.77	Joback Method
dvisc	0.0021076	Pa×s	260.82	Joback Method
dvisc	0.0012789	Pa×s	296.47	Joback Method
dvisc	0.0008639	Pa×s	332.11	Joback Method
dvisc	0.0006296	Pa×s	367.76	Joback Method
dvisc	0.0004853	Pa×s	403.41	Joback Method
dvisc	0.0003902	Pa×s	439.05	Joback Method
dvisc	0.0003242	Pa×s	474.70	Joback Method

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=C3365262&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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