Benzene, cyclobutyl-

Other names: Cyclobutane, phenyl-
Cyclobutylbenzene
Phenylcyclobutane
Inchi: InChI=1S/C10H12/c1-2-5-9(6-3-1)10-7-4-8-10/h1-3,5-6,10H,4,7-8H2
InchiKey: UJMBCHVRTIOTKC-UHFFFAOYSA-N
Formula: C10H12
SMILES: c1ccc(C2CCC2)cc1
Mol. weight [g/mol]: 132.20
CAS: 4392-30-7

Physical Properties

Property code	Value	Unit	Source
gf	194.38	kJ/mol	Joback Method
hf	53.44	kJ/mol	Joback Method
hfus	11.73	kJ/mol	Joback Method
hvap	40.22	kJ/mol	Joback Method
ie	8.40	eV	NIST Webbook
ie	8.77	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
ie	8.77	eV	NIST Webbook
log10ws	-2.97		Crippen Method
logp	2.954		Crippen Method
mcvol	117.140	ml/mol	McGowan Method
pc	3493.01	kPa	Joback Method
tb	465.89	K	Joback Method
tc	696.83	K	Joback Method
tf	243.30	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.06	J/mol×K	465.89	Joback Method
cpg	317.06	J/mol×K	658.34	Joback Method

cpg	304.06	J/mol×K	619.85	Joback Method
cpg	290.03	J/mol×K	581.36	Joback Method
cpg	274.90	J/mol×K	542.87	Joback Method
cpg	258.60	J/mol×K	504.38	Joback Method
cpg	329.10	J/mol×K	696.83	Joback Method
dvisc	0.0003531	Pa×s	465.89	Joback Method
dvisc	0.0004238	Pa×s	428.79	Joback Method
dvisc	0.0005266	Pa×s	391.69	Joback Method
dvisc	0.0006847	Pa×s	354.60	Joback Method
dvisc	0.0009467	Pa×s	317.50	Joback Method
dvisc	0.0014259	Pa×s	280.40	Joback Method
dvisc	0.0024336	Pa×s	243.30	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4392307&Units=SI
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

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