Cyclobutadiene

Inchi: InChI=1S/C4H4/c1-2-4-3-1/h1-4H
InchiKey: HWEQKSVYKBUIIK-UHFFFAOYSA-N
Formula: C4H4
SMILES: C1=CC=C1
Mol. weight [g/mol]: 52.07
CAS: 1120-53-2

Physical Properties

Property code	Value	Unit	Source
gf	99.08	kJ/mol	Joback Method
hf	76.65	kJ/mol	Joback Method
hfus	3.52	kJ/mol	Joback Method
hvap	25.48	kJ/mol	Joback Method
ie	8.24	eV	NIST Webbook
ie	8.16 ± 0.03	eV	NIST Webbook
ie	9.55	eV	NIST Webbook
ie	8.20	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
log10ws	-1.10		Crippen Method
logp	1.112		Crippen Method
mcvol	47.760	ml/mol	McGowan Method
pc	5552.58	kPa	Joback Method
tb	304.92	K	Joback Method
tc	496.15	K	Joback Method
tf	155.02	K	Joback Method
vc	0.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	54.63	J/mol×K	304.92	Joback Method
cpg	61.91	J/mol×K	336.79	Joback Method
cpg	68.68	J/mol×K	368.66	Joback Method
cpg	74.96	J/mol×K	400.53	Joback Method

cpg	80.77	J/mol×K	432.40	Joback Method
cpg	86.16	J/mol×K	464.28	Joback Method
cpg	91.14	J/mol×K	496.15	Joback Method
dvisc	0.0007363	Pa×s	155.02	Joback Method
dvisc	0.0004962	Pa×s	180.00	Joback Method
dvisc	0.0003682	Pa×s	204.99	Joback Method
dvisc	0.0002915	Pa×s	229.97	Joback Method
dvisc	0.0002416	Pa×s	254.95	Joback Method
dvisc	0.0002070	Pa×s	279.94	Joback Method
dvisc	0.0001820	Pa×s	304.92	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1120532&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

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