Cyclopropenyl radical

Inchi: InChI=1S/C3H3/c1-2-3-1/h1-3H
InchiKey: UKPXULFIISGBHG-UHFFFAOYSA-N
Formula: C3H3
SMILES: [CH]1C=C1
Mol. weight [g/mol]: 39.06
CAS: 28933-84-8

Physical Properties

Property code	Value	Unit	Source
affp	734.30	kJ/mol	NIST Webbook
basg	701.80	kJ/mol	NIST Webbook
gf	117.47	kJ/mol	Joback Method
hf	81.14	kJ/mol	Joback Method
hfpi	1080.00	kJ/mol	NIST Webbook
hfus	4.57	kJ/mol	Joback Method
hvap	22.33	kJ/mol	Joback Method
ie	6.60	eV	NIST Webbook
log10ws	-0.44		Crippen Method
logp	0.760		Crippen Method
mcvol	35.820	ml/mol	McGowan Method
pc	5953.74	kPa	Joback Method
tb	273.24	K	Joback Method
tc	447.36	K	Joback Method
tf	158.64	K	Joback Method
vc	0.138	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	33.75	J/mol×K	273.24	Joback Method
cpg	40.32	J/mol×K	302.26	Joback Method
cpg	46.33	J/mol×K	331.28	Joback Method
cpg	51.80	J/mol×K	360.30	Joback Method
cpg	56.76	J/mol×K	389.32	Joback Method

cpg	61.26	J/mol×K	418.34	Joback Method
cpg	65.32	J/mol×K	447.36	Joback Method
dvisc	0.0000232	Pa×s	158.64	Joback Method
dvisc	0.0000320	Pa×s	177.74	Joback Method
dvisc	0.0000414	Pa×s	196.84	Joback Method
dvisc	0.0000512	Pa×s	215.94	Joback Method
dvisc	0.0000612	Pa×s	235.04	Joback Method
dvisc	0.0000712	Pa×s	254.14	Joback Method
dvisc	0.0000811	Pa×s	273.24	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=C28933848&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfpi: Enthalpy of formation of positive ion 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