Methylenecyclopropane

Other names: Cyclopropane, methylene-
Inchi: InChI=1S/C4H6/c1-4-2-3-4/h1-3H2
InchiKey: XSGHLZBESSREDT-UHFFFAOYSA-N
Formula: C4H6
SMILES: C=C1CC1
Mol. weight [g/mol]: 54.09
CAS: 6142-73-0

Physical Properties

Property code	Value	Unit	Source
chg	-2632.00 ± 1.90	kJ/mol	NIST Webbook
gf	104.34	kJ/mol	Joback Method
hf	201.00 ± 2.00	kJ/mol	NIST Webbook
hfus	2.02	kJ/mol	Joback Method
hvap	24.88	kJ/mol	Joback Method
ie	9.57	eV	NIST Webbook
ie	9.60 ± 0.10	eV	NIST Webbook
log10ws	-1.25		Crippen Method
logp	1.336		Crippen Method
mcvol	52.060	ml/mol	McGowan Method
pc	4959.33	kPa	Joback Method
rinpol	432.50		NIST Webbook
rinpol	432.00		NIST Webbook
rinpol	432.50		NIST Webbook
tb	301.49	K	Joback Method
tc	481.67	K	Joback Method
tf	134.50 ± 1.00	K	NIST Webbook
tf	137.00 ± 1.00	K	NIST Webbook
vc	0.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	68.56	J/mol×K	301.49	Joback Method

cpg	75.93	J/mol×K	331.52	Joback Method
cpg	82.87	J/mol×K	361.55	Joback Method
cpg	89.39	J/mol×K	391.58	Joback Method
cpg	95.52	J/mol×K	421.61	Joback Method
cpg	101.27	J/mol×K	451.64	Joback Method
cpg	106.67	J/mol×K	481.67	Joback Method
dvisc	0.0003809	Pa×s	170.70	Joback Method
dvisc	0.0003192	Pa×s	192.50	Joback Method
dvisc	0.0002772	Pa×s	214.30	Joback Method
dvisc	0.0002472	Pa×s	236.09	Joback Method
dvisc	0.0002247	Pa×s	257.89	Joback Method
dvisc	0.0002073	Pa×s	279.69	Joback Method
dvisc	0.0001935	Pa×s	301.49	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6142730&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

chg: Standard gas enthalpy of combustion
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume