Bicyclo[1.1.0]but-1(3)-ene

Inchi: InChI=1S/C4H4/c1-3-2-4(1)3/h1-2H2
InchiKey: JTVNFJINIGKHAV-UHFFFAOYSA-N
Formula: C4H4
SMILES: C1C2=C1C2
Mol. weight [g/mol]: 52.07
CAS: 58208-49-4

Physical Properties

Property code	Value	Unit	Source
ea	0.35 ± 0.17	eV	NIST Webbook
gf	154.62	kJ/mol	Joback Method
hf	544.00 ± 42.00	kJ/mol	NIST Webbook
hfus	4.89	kJ/mol	Joback Method
hvap	26.21	kJ/mol	Joback Method
log10ws	-1.14		Crippen Method
logp	1.090		Crippen Method
mcvol	41.200	ml/mol	McGowan Method
pc	5739.21	kPa	Joback Method
tb	314.32	K	Joback Method
tc	500.08	K	Joback Method
tf	212.04	K	Joback Method
vc	0.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	57.92	J/mol×K	314.32	Joback Method
cpg	86.39	J/mol×K	469.12	Joback Method
cpg	81.92	J/mol×K	438.16	Joback Method
cpg	76.88	J/mol×K	407.20	Joback Method
cpg	71.24	J/mol×K	376.24	Joback Method
cpg	64.94	J/mol×K	345.28	Joback Method
cpg	90.37	J/mol×K	500.08	Joback Method
dvisc	0.0001974	Pa×s	314.32	Joback Method

dvisc	0.0001811	Pa×s	297.27	Joback Method
dvisc	0.0001643	Pa×s	280.23	Joback Method
dvisc	0.0001473	Pa×s	263.18	Joback Method
dvisc	0.0001300	Pa×s	246.13	Joback Method
dvisc	0.0001126	Pa×s	229.09	Joback Method
dvisc	0.0000954	Pa×s	212.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58208494&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
ea:	Electron affinity
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
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