Bicyclo[1.1.0]butane

Inchi: InChI=1S/C4H6/c1-3-2-4(1)3/h3-4H,1-2H2
InchiKey: LASLVGACQUUOEB-UHFFFAOYSA-N
Formula: C4H6
SMILES: C1C2CC12
Mol. weight [g/mol]: 54.09
CAS: 157-33-5

Physical Properties

Property code	Value	Unit	Source
chg	-2648.70 ± 0.79	kJ/mol	NIST Webbook
gf	128.50	kJ/mol	Joback Method
hf	217.00 ± 0.80	kJ/mol	NIST Webbook
hfus	6.59	kJ/mol	Joback Method
hvap	23.98	kJ/mol	Joback Method
ie	8.70 ± 0.01	eV	NIST Webbook
ie	8.70 ± 0.01	eV	NIST Webbook
log10ws	-0.80		Crippen Method
logp	1.026		Crippen Method
mcvol	45.500	ml/mol	McGowan Method
pc	5160.85	kPa	Joback Method
tb	281.40	K	NIST Webbook
tc	473.47	K	Joback Method
tf	177.76	K	Joback Method
vc	0.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	61.53	J/mol×K	295.86	Joback Method
cpg	104.40	J/mol×K	443.87	Joback Method
cpg	97.18	J/mol×K	414.27	Joback Method
cpg	89.33	J/mol×K	384.67	Joback Method
cpg	80.80	J/mol×K	355.06	Joback Method
cpg	71.55	J/mol×K	325.46	Joback Method

cpg	111.03	J/mol×K	473.47	Joback Method
dvisc	0.0001347	Pa×s	295.86	Joback Method
dvisc	0.0001119	Pa×s	276.18	Joback Method
dvisc	0.0000903	Pa×s	256.49	Joback Method
dvisc	0.0000703	Pa×s	236.81	Joback Method
dvisc	0.0000523	Pa×s	217.13	Joback Method
dvisc	0.0000367	Pa×s	197.44	Joback Method
dvisc	0.0000238	Pa×s	177.76	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C157335&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume