

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

Physical Properties

Property code	Value	Unit	Source
chg	-2648.70 ± 0.79	kJ/mol	NIST Webbook
hf	217.00 ± 0.80	kJ/mol	NIST Webbook
hfus	6.59	kJ/mol	Joback Method
hvap	20.79	kJ/mol	Cheméo Relay (1.0)
ie	8.70 ± 0.01	eV	NIST Webbook
ie	8.70 ± 0.01	eV	NIST Webbook
logp	1.026		Crippen Method
mcvol	45.500	ml/mol	McGowan Method
tb	281.40	K	NIST Webbook
tf	259.05	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	61.53	J/mol×K	295.86	Joback Method
cpg	71.55	J/mol×K	325.46	Joback Method
cpg	80.80	J/mol×K	355.06	Joback Method
cpg	89.33	J/mol×K	384.67	Joback Method
cpg	97.18	J/mol×K	414.27	Joback Method
cpg	104.40	J/mol×K	443.87	Joback Method
cpg	111.03	J/mol×K	473.47	Joback Method
dvisc	0.0000238	Pa×s	177.76	Joback Method
dvisc	0.0000367	Pa×s	197.44	Joback Method
dvisc	0.0000523	Pa×s	217.13	Joback Method
dvisc	0.0000703	Pa×s	236.81	Joback Method
dvisc	0.0000903	Pa×s	256.49	Joback Method

dvisc	0.0001119	Pa×s	276.18	Joback Method
dvisc	0.0001347	Pa×s	295.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C157335&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chg:	Standard gas enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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