

2-Methylbicyclo[2.2.2]octane

Other names:	2-methylbicyclo[2.2.2]octane
Inchi:	InChI=1S/C9H16/c1-7-6-8-2-4-9(7)5-3-8/h7-9H,2-6H2,1H3
InchiKey:	WNPVIRUJGYEGOJ-UHFFFAOYSA-N
Formula:	C9H16
SMILES:	CC1CC2CCC1CC2
Mol. weight [g/mol]:	124.23

Physical Properties

Property code	Value	Unit	Source
hf	-107.62	kJ/mol	Cheméo Relay (1.0)
hfus	12.21	kJ/mol	Joback Method
ie	9.24	eV	Cheméo Relay (1.0)
logp	2.833		Crippen Method
mcvol	115.950	ml/mol	McGowan Method
tb	432.61	K	Cheméo Relay (1.0)
tf	327.01	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.34	J/mol×K	422.67	Joback Method
cpg	260.95	J/mol×K	457.20	Joback Method
cpg	279.43	J/mol×K	491.74	Joback Method
cpg	296.83	J/mol×K	526.27	Joback Method
cpg	313.20	J/mol×K	560.81	Joback Method
cpg	328.59	J/mol×K	595.34	Joback Method
cpg	343.05	J/mol×K	629.88	Joback Method
dvisc	0.0009865	Pa×s	215.79	Joback Method
dvisc	0.0008118	Pa×s	250.27	Joback Method
dvisc	0.0007004	Pa×s	284.75	Joback Method
dvisc	0.0006238	Pa×s	319.23	Joback Method
dvisc	0.0005683	Pa×s	353.71	Joback Method
dvisc	0.0005263	Pa×s	388.19	Joback Method
dvisc	0.0004936	Pa×s	422.67	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C766530&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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):

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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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