Bicyclo[2.2.2]octane, 1-methoxy-4-methyl-

Other names: 1-methoxy-4-methyl-bicyclo[2.2.2]octane
Inchi: InChI=1S/C10H18O/c1-9-3-6-10(11-2,7-4-9)8-5-9/h3-8H2,1-2H3
InchiKey: NXGYBOISDZEYCB-UHFFFAOYSA-N
Formula: C10H18O
SMILES: COC12CCC(C)(CC1)CC2
Mol. weight [g/mol]: 154.25
CAS: 6555-95-9

Physical Properties

Property code	Value	Unit	Source
gf	14.64	kJ/mol	Joback Method
hf	-218.19	kJ/mol	Joback Method
hfus	2.32	kJ/mol	Joback Method
hvap	38.13	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	2.746		Crippen Method
mcvol	135.910	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
rinpol	1341.00		NIST Webbook
rinpol	1341.00		NIST Webbook
tb	473.12	K	Joback Method
tc	695.18	K	Joback Method
tf	301.33	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.47	J/mol×K	473.12	Joback Method
cpg	335.35	J/mol×K	510.13	Joback Method
cpg	353.54	J/mol×K	547.14	Joback Method
cpg	370.27	J/mol×K	584.15	Joback Method
cpg	385.80	J/mol×K	621.16	Joback Method
cpg	400.36	J/mol×K	658.17	Joback Method

cpg	414.19	J/mol×K	695.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6555959&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume