Bicyclo[2.2.1]hept-2-ene,5-methoxy-, exo-

Inchi:	InChI=1S/C8H12O/c1-9-8-5-6-2-3-7(8)4-6/h2-3,6-8H,4-5H2,1H3/t6?,7?,8-/m0/s1
InchiKey:	RCDOWRWNYHNLLA-RRQHEKLDSA-N
Formula:	C8H12O
SMILES:	COC1CC2C=CC1C2
Mol. weight [g/mol]:	124.18
CAS:	17190-87-3

Physical Properties

Property code	Value	Unit	Source
gf	43.13	kJ/mol	Joback Method
hf	-163.79	kJ/mol	Joback Method
hfus	14.13	kJ/mol	Joback Method
hvap	35.79	kJ/mol	Joback Method
ie	8.68 ± 0.03	eV	NIST Webbook
log10ws	-1.53		Crippen Method
logp	1.597		Crippen Method
mcvol	103.430	ml/mol	McGowan Method
pc	3399.94	kPa	Joback Method
tb	417.10	K	Joback Method
tc	619.33	K	Joback Method
tf	231.03	K	Joback Method
vc	0.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.59	J/mol×K	417.10	Joback Method
cpg	228.26	J/mol×K	450.81	Joback Method
cpg	243.05	J/mol×K	484.51	Joback Method
cpg	256.99	J/mol×K	518.22	Joback Method
cpg	270.12	J/mol×K	551.92	Joback Method
cpg	282.48	J/mol×K	585.63	Joback Method
cpg	294.11	J/mol×K	619.33	Joback Method
dvisc	0.0004866	Pa×s	231.03	Joback Method

dvisc	0.0004806	Pa×s	262.04	Joback Method
dvisc	0.0004760	Pa×s	293.05	Joback Method
dvisc	0.0004722	Pa×s	324.07	Joback Method
dvisc	0.0004692	Pa×s	355.08	Joback Method
dvisc	0.0004666	Pa×s	386.09	Joback Method
dvisc	0.0004645	Pa×s	417.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17190873&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
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

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