

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

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-/m1/s1
InchiKey:	RCDOWRWNYHNLLA-KAVNDROISA-N
Formula:	C8H12O
SMILES:	COC1CC2C=CC1C2
Mol. weight [g/mol]:	124.18
CAS:	17190-92-0

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	8.69 ± 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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.59	J/molxK	417.10	Joback Method
cpg	282.48	J/molxK	585.63	Joback Method
cpg	270.12	J/molxK	551.92	Joback Method
cpg	256.99	J/molxK	518.22	Joback Method
cpg	243.05	J/molxK	484.51	Joback Method
cpg	228.26	J/molxK	450.81	Joback Method
cpg	294.11	J/molxK	619.33	Joback Method
dvisc	0.0004645	Paxs	417.10	Joback Method

dvisc	0.0004666	Paxs	386.09	Joback Method
dvisc	0.0004692	Paxs	355.08	Joback Method
dvisc	0.0004722	Paxs	324.07	Joback Method
dvisc	0.0004760	Paxs	293.05	Joback Method
dvisc	0.0004806	Paxs	262.04	Joback Method
dvisc	0.0004866	Paxs	231.03	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17190920&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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