Bicyclo[3.2.0]hept-2-en-6-one

Other names: cis-Bicyclo[3.2.0]heptane
Inchi: InChI=1S/C7H8O/c8-7-4-5-2-1-3-6(5)7/h1-2,5-6H,3-4H2
InchiKey: LNLLHUHPGPKRBM-UHFFFAOYSA-N
Formula: C7H8O
SMILES: O=C1CC2C=CCC12
Mol. weight [g/mol]: 108.14
CAS: 13173-09-6

Physical Properties

Property code	Value	Unit	Source
gf	24.83	kJ/mol	Joback Method
hf	-128.29	kJ/mol	Joback Method
hfus	8.79	kJ/mol	Joback Method
hvap	35.71	kJ/mol	Joback Method
log10ws	-1.19		Crippen Method
logp	1.151		Crippen Method
mcvol	85.040	ml/mol	McGowan Method
pc	4249.61	kPa	Joback Method
rinpol	787.00		NIST Webbook
tb	444.29	K	Joback Method
tc	671.01	K	Joback Method
tf	269.99	K	Joback Method
vc	0.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.45	J/mol×K	444.29	Joback Method
cpg	190.19	J/mol×K	482.08	Joback Method
cpg	203.08	J/mol×K	519.86	Joback Method
cpg	215.13	J/mol×K	557.65	Joback Method
cpg	226.41	J/mol×K	595.44	Joback Method
cpg	236.95	J/mol×K	633.22	Joback Method
cpg	246.79	J/mol×K	671.01	Joback Method

Sources

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=C13173096&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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