2-Oxabicyclo[2.2.0]hex-5-en-3-one

Other names: 2-Oxa-3-oxobicyclo[2.2.0]hex-5-ene
Inchi: InChI=1S/C5H4O2/c6-5-3-1-2-4(3)7-5/h1-4H
InchiKey: QAVYTTBRXJVSNJ-UHFFFAOYSA-N
Formula: C5H4O2
SMILES: O=C1OC2C=CC12
Mol. weight [g/mol]: 96.08
CAS: 22980-23-0

Physical Properties

Property code	Value	Unit	Source
gf	-66.03	kJ/mol	Joback Method
hf	-212.85	kJ/mol	Joback Method
hfus	13.69	kJ/mol	Joback Method
hvap	35.60	kJ/mol	Joback Method
log10ws	-0.29		Crippen Method
logp	0.098		Crippen Method
mcvol	62.730	ml/mol	McGowan Method
pc	5281.57	kPa	Joback Method
tb	421.21	K	Joback Method
tc	644.06	K	Joback Method
tf	277.54	K	Joback Method
vc	0.243	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	127.96	J/mol×K	421.21	Joback Method
cpg	137.64	J/mol×K	458.35	Joback Method
cpg	146.67	J/mol×K	495.49	Joback Method
cpg	155.07	J/mol×K	532.63	Joback Method
cpg	162.89	J/mol×K	569.78	Joback Method
cpg	170.16	J/mol×K	606.92	Joback Method
cpg	176.94	J/mol×K	644.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22980230&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume