Cyclopentanone, 3,4-bis(methylene)-

Inchi: InChI=1S/C7H8O/c1-5-3-7(8)4-6(5)2/h1-4H2
InchiKey: QLTBRYOQIIJWSI-UHFFFAOYSA-N
Formula: C7H8O
SMILES: C=C1CC(=O)CC1=C
Mol. weight [g/mol]: 108.14
CAS: 27646-73-7

Physical Properties

Property code	Value	Unit	Source
gf	35.89	kJ/mol	Joback Method
hf	-76.21	kJ/mol	Joback Method
hfus	3.94	kJ/mol	Joback Method
hvap	36.31	kJ/mol	Joback Method
log10ws	-1.63		Crippen Method
logp	1.462		Crippen Method
mcvol	91.600	ml/mol	McGowan Method
pc	3886.79	kPa	Joback Method
ripol	2384.00		NIST Webbook
tb	445.65	K	Joback Method
tc	664.96	K	Joback Method
tf	279.37	K	Joback Method
vc	0.344	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.11	J/mol×K	445.65	Joback Method
cpg	186.09	J/mol×K	482.20	Joback Method
cpg	196.65	J/mol×K	518.75	Joback Method
cpg	206.79	J/mol×K	555.30	Joback Method
cpg	216.49	J/mol×K	591.85	Joback Method
cpg	225.74	J/mol×K	628.41	Joback Method
cpg	234.54	J/mol×K	664.96	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=C27646737&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume