cyclohex-3-en-1-one

Inchi: InChI=1S/C6H8O/c7-6-4-2-1-3-5-6/h1-2H,3-5H2
InchiKey: VNLZLLDMKRKVEX-UHFFFAOYSA-N
Formula: C6H8O
SMILES: O=C1CC=CCC1
Mol. weight [g/mol]: 96.13
CAS: 4096-34-8

Physical Properties

Property code	Value	Unit	Source
gf	-60.83	kJ/mol	Joback Method
hf	-172.43	kJ/mol	Joback Method
hfus	2.79	kJ/mol	Joback Method
hvap	34.23	kJ/mol	Joback Method
ie	9.42	eV	NIST Webbook
log10ws	-1.36		Crippen Method
logp	1.296		Crippen Method
mcvol	81.810	ml/mol	McGowan Method
pc	4534.68	kPa	Joback Method
tb	427.88	K	Joback Method
tc	657.68	K	Joback Method
tf	237.98	K	Joback Method
vc	0.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.01	J/mol×K	427.88	Joback Method
cpg	161.60	J/mol×K	466.18	Joback Method
cpg	173.60	J/mol×K	504.48	Joback Method
cpg	185.03	J/mol×K	542.78	Joback Method
cpg	195.87	J/mol×K	581.08	Joback Method
cpg	206.12	J/mol×K	619.38	Joback Method
cpg	215.77	J/mol×K	657.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4096348&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
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