2-Cycloocten-1-one

Other names: 2-Cyclooctenone
Inchi: InChI=1S/C8H12O/c9-8-6-4-2-1-3-5-7-8/h4,6H,1-3,5,7H2/b6-4-
InchiKey: NSHQAIKRVDXIMX-XQRVVYSFSA-N
Formula: C8H12O
SMILES: O=C1C=CCCCCC1
Mol. weight [g/mol]: 124.18
CAS: 1728-25-2

Physical Properties

Property code	Value	Unit	Source
gf	-68.19	kJ/mol	Joback Method
hf	-226.03	kJ/mol	Joback Method
hfus	3.77	kJ/mol	Joback Method
hvap	39.02	kJ/mol	Joback Method
ie	9.18	eV	NIST Webbook
log10ws	-2.20		Crippen Method
logp	2.076		Crippen Method
mcvol	109.990	ml/mol	McGowan Method
pc	3777.68	kPa	Joback Method
tb	482.18	K	Joback Method
tc	723.46	K	Joback Method
tf	253.48	K	Joback Method
vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.22	J/mol×K	482.18	Joback Method
cpg	246.69	J/mol×K	522.39	Joback Method
cpg	263.27	J/mol×K	562.61	Joback Method
cpg	278.96	J/mol×K	602.82	Joback Method
cpg	293.73	J/mol×K	643.03	Joback Method
cpg	307.57	J/mol×K	683.24	Joback Method
cpg	320.46	J/mol×K	723.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1728252&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