Cyclohexanone, 2-cyclohexylidene-

Other names:	Bicyclohexyliden-2-one
	Dianon
	2-Cyclohexylidenecyclohexanone
Inchi:	InChI=1S/C12H18O/c13-12-9-5-4-8-11(12)10-6-2-1-3-7-10/h1-9H2
InchiKey:	TYDSIOSLHQWFOU-UHFFFAOYSA-N
Formula:	C12H18O
SMILES:	O=C1CCCCC1=C1CCCCC1
Mol. weight [g/mol]:	178.27
CAS:	1011-12-7

Physical Properties

Property code	Value	Unit	Source
chs	-6987.70 ± 1.20	kJ/mol	NIST Webbook
gf	2.59	kJ/mol	Joback Method
hf	-213.80 ± 2.40	kJ/mol	NIST Webbook
hfs	-307.00 ± 2.00	kJ/mol	NIST Webbook
hfus	8.32	kJ/mol	Joback Method
hvap	49.64	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.390		Crippen Method
mcvol	155.490	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
tb	599.34	K	Joback Method
tc	851.04	K	Joback Method
tf	342.26	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.50	J/mol×K	599.34	Joback Method
cpg	428.31	J/mol×K	641.29	Joback Method
cpg	448.65	J/mol×K	683.24	Joback Method
cpg	467.54	J/mol×K	725.19	Joback Method

cpg	485.00	J/mol×K	767.14	Joback Method
cpg	501.06	J/mol×K	809.09	Joback Method
cpg	515.74	J/mol×K	851.04	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1011127&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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

Latest version available from:
https://www.chemeo.com/cid/60-115-7/Cyclohexanone-2-cyclohexylidene.pdf
Generated by Cheméo on 2024-10-12 04:26:49.472350961 +0000 UTC m=+3288072.109320208.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.