

2-(1-Cyclohexenyl)cyclohexanone

Other names:	Cyclohexanone, 2-(1-cyclohexen-1-yl)- CHCH 2-(Cyclohex-1-enyl)cyclohexanone 2-(1-Cyclohexen-1-yl)cyclohexanone 2-Cyclohexenylcyclohexanone 2-(1-cyclohexen-1-yl)cyclohexan-1-one
Inchi:	InChI=1S/C12H18O/c13-12-9-5-4-8-11(12)10-6-2-1-3-7-10/h6,11H,1-5,7-9H2
InchiKey:	GVNVAWHJIKLAGL-UHFFFAOYSA-N
Formula:	C12H18O
SMILES:	O=C1CCCCC1C1=CCCCC1
Mol. weight [g/mol]:	178.27
CAS:	1502-22-3

Physical Properties

Property code	Value	Unit	Source
chl	-7005.87 ± 0.74	kJ/mol	NIST Webbook
gf	4.51	kJ/mol	Joback Method
hf	-219.50 ± 1.80	kJ/mol	NIST Webbook
hfl	-288.80 ± 1.80	kJ/mol	NIST Webbook
hfus	9.78	kJ/mol	Joback Method
hvap	48.67	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.246		Crippen Method
mvol	155.490	ml/mol	McGowan Method
pc	2856.62	kPa	Joback Method
tb	589.69	K	Joback Method
tc	840.48	K	Joback Method
tf	325.50	K	Joback Method
vc	0.568	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.65	J/mol×K	589.69	Joback Method

cpg	430.35	J/mol×K	631.49	Joback Method
cpg	451.53	J/mol×K	673.29	Joback Method
cpg	471.20	J/mol×K	715.08	Joback Method
cpg	489.38	J/mol×K	756.88	Joback Method
cpg	506.10	J/mol×K	798.68	Joback Method
cpg	521.37	J/mol×K	840.48	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	416.00 ± 1.00	K	2.00	NIST Webbook

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=C1502223&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid 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
tbrp:	Boiling point at reduced pressure

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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