[1,1'-Bicyclohexyl]-2-one

Other names: Cyclohexanone, 2-cyclohexyl-
Lavamenthe
2-Cyclohexylcyclohexanone
Inchi: InChI=1S/C12H20O/c13-12-9-5-4-8-11(12)10-6-2-1-3-7-10/h10-11H,1-9H2
InchiKey: UOBQDYFTAJKQAL-UHFFFAOYSA-N
Formula: C12H20O
SMILES: O=C1CCCCC1C1CCCCC1
Mol. weight [g/mol]: 180.29
CAS: 90-42-6

Physical Properties

Property code	Value	Unit	Source
chs	-7189.49 ± 0.98	kJ/mol	NIST Webbook
gf	-23.53	kJ/mol	Joback Method
hf	-324.00 ± 1.50	kJ/mol	NIST Webbook
hfs	-391.00 ± 1.40	kJ/mol	NIST Webbook
hfus	10.02	kJ/mol	Joback Method
hvap	47.41	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.326		Crippen Method
mcvol	159.790	ml/mol	McGowan Method
pc	2698.60	kPa	Joback Method
rinpol	1496.00		NIST Webbook
rinpol	1496.00		NIST Webbook
ripol	1975.00		NIST Webbook
tb	580.88	K	Joback Method
tc	787.00 ± 35.00	K	NIST Webbook
tf	307.98	K	Joback Method
tt	277.00 ± 1.00	K	NIST Webbook
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	536.71	J/mol×K	786.95	Joback Method
cpg	428.54	J/mol×K	580.88	Joback Method
cpg	453.38	J/mol×K	622.09	Joback Method
cpg	476.60	J/mol×K	663.31	Joback Method
cpg	498.22	J/mol×K	704.52	Joback Method
cpg	518.25	J/mol×K	745.73	Joback Method
cpg	553.62	J/mol×K	828.16	Joback Method
hfust	18.00	kJ/mol	277.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C90426&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
hfust: Enthalpy of fusion at a given temperature
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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
tt: Triple Point Temperature
vc: Critical Volume