Methanone, dicyclohexyl-

Other names:	Cyclohexyl ketone
	Cyclohexane ketone
	Dicyclohexyl ketone
	Ketone, dicyclohexyl
Inchi:	InChI=1S/C13H22O/c14-13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h11-12H,1-10H2
InchiKey:	TWXWPPKDQOWNSX-UHFFFAOYSA-N
Formula:	C13H22O
SMILES:	O=C(C1CCCCC1)C1CCCCC1
Mol. weight [g/mol]:	194.31
CAS:	119-60-8

Physical Properties

Property code	Value	Unit	Source
gf	-21.44	kJ/mol	Joback Method
hf	-315.59	kJ/mol	Joback Method
hfus	14.69	kJ/mol	Joback Method
hvap	52.14	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.716		Crippen Method
mcvol	173.880	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
rinpol	1576.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	1576.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1565.00		NIST Webbook
ripol	1957.00		NIST Webbook
ripol	1883.00		NIST Webbook
ripol	1920.00		NIST Webbook
tb	589.81	K	Joback Method
tc	825.67	K	Joback Method
tf	300.96	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.33	J/mol×K	589.81	Joback Method
cpg	493.65	J/mol×K	629.12	Joback Method
cpg	516.31	J/mol×K	668.43	Joback Method
cpg	537.36	J/mol×K	707.74	Joback Method
cpg	556.87	J/mol×K	747.05	Joback Method
cpg	574.89	J/mol×K	786.36	Joback Method
cpg	591.48	J/mol×K	825.67	Joback Method
dvisc	0.0066183	Pa×s	300.96	Joback Method
dvisc	0.0026118	Pa×s	349.10	Joback Method
dvisc	0.0012912	Pa×s	397.24	Joback Method
dvisc	0.0007434	Pa×s	445.38	Joback Method
dvisc	0.0004766	Pa×s	493.53	Joback Method
dvisc	0.0003307	Pa×s	541.67	Joback Method
dvisc	0.0002436	Pa×s	589.81	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	411.20	K	1.70	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C119608&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
dvisc:	Dynamic viscosity
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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume