Phenyl cyclohexyl ketone

Other names:	Methanone, cyclohexylphenyl-
	Ketone, cyclohexyl phenyl
	Benzophenone, 1,2,3,4,5,6-hexahydro-
	Benzoyl cyclohexane
	Cyclohexyl phenyl ketone
	USAF KF-3
Inchi:	InChI=1S/C13H16O/c14-13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1,3-4,7-8,12H,2,5-6,9-10
InchiKey:	BMFYCFSWWDXEPB-UHFFFAOYSA-N
Formula:	C13H16O
SMILES:	O=C(c1ccccc1)C1CCCCC1
Mol. weight [g/mol]:	188.27
CAS:	712-50-5

Physical Properties

Property code	Value	Unit	Source
gf	66.52	kJ/mol	Joback Method
hf	-133.38	kJ/mol	Joback Method
hfus	16.90	kJ/mol	Joback Method
hvap	53.98	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.450		Crippen Method
mcvol	160.980	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
rinpol	1608.00		NIST Webbook
tb	596.94	K	Joback Method
tc	840.91	K	Joback Method
tf	332.50 ± 0.50	K	NIST Webbook
vc	0.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.71	J/mol×K	596.94	Joback Method
cpg	426.59	J/mol×K	637.60	Joback Method

cpg	444.96	J/mol×K	678.26	Joback Method
cpg	461.91	J/mol×K	718.92	Joback Method
cpg	477.50	J/mol×K	759.58	Joback Method
cpg	491.80	J/mol×K	800.24	Joback Method
cpg	504.88	J/mol×K	840.91	Joback Method
dvisc	0.0037215	Pa×s	320.00	Joback Method
dvisc	0.0017342	Pa×s	366.16	Joback Method
dvisc	0.0009588	Pa×s	412.31	Joback Method
dvisc	0.0005973	Pa×s	458.47	Joback Method
dvisc	0.0004057	Pa×s	504.63	Joback Method
dvisc	0.0002940	Pa×s	550.78	Joback Method
dvisc	0.0002240	Pa×s	596.94	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	437.70	K	2.40	NIST Webbook
tbrp	428.00 ± 2.00	K	2.00	NIST Webbook
tbrp	437.50 ± 0.50	K	2.40	NIST Webbook

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=C712505&Units=SI

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
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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