Cyclopropyl phenyl ketone

Other names:	Methanone, cyclopropylphenyl-
	Ketone, cyclopropyl phenyl
	Benzoylcyclopropane
	Phenyl cyclopropyl ketone
	Cyclopropylphenylmethanone
Inchi:	InChI=1S/C10H10O/c11-10(9-6-7-9)8-4-2-1-3-5-8/h1-5,9H,6-7H2
InchiKey:	PJRHFTYXYCVOSJ-UHFFFAOYSA-N
Formula:	C10H10O
SMILES:	O=C(c1ccccc1)C1CC1
Mol. weight [g/mol]:	146.19
CAS:	3481-02-5

Physical Properties

Property code	Value	Unit	Source
gf	77.56	kJ/mol	Joback Method
hf	-52.98	kJ/mol	Joback Method
hfus	15.43	kJ/mol	Joback Method
hvap	46.79	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.279		Crippen Method
mcvol	118.710	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
rinpol	1270.00		NIST Webbook
tb	515.49	K	Joback Method
tc	747.78	K	Joback Method
tf	296.75	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.92	J/mol×K	515.49	Joback Method
cpg	276.80	J/mol×K	554.21	Joback Method
cpg	290.54	J/mol×K	592.92	Joback Method

cpg	303.21	J/mol×K	631.64	Joback Method
cpg	314.90	J/mol×K	670.35	Joback Method
cpg	325.68	J/mol×K	709.07	Joback Method
cpg	335.62	J/mol×K	747.78	Joback Method
dvisc	0.0022723	Pa×s	296.75	Joback Method
dvisc	0.0015624	Pa×s	333.21	Joback Method
dvisc	0.0011567	Pa×s	369.66	Joback Method
dvisc	0.0009039	Pa×s	406.12	Joback Method
dvisc	0.0007356	Pa×s	442.58	Joback Method
dvisc	0.0006177	Pa×s	479.03	Joback Method
dvisc	0.0005316	Pa×s	515.49	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	395.20	K	2.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3481025&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

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