Methanone, dicyclopropyl-

Other names:	Cyclopropyl ketone
	Dicyclopropyl ketone
	Dicyclopropylmethanone
Inchi:	InChI=1S/C7H10O/c8-7(5-1-2-5)6-3-4-6/h5-6H,1-4H2
InchiKey:	BIPUHAHGLJKIPK-UHFFFAOYSA-N
Formula:	C7H10O
SMILES:	O=C(C1CC1)C1CC1
Mol. weight [g/mol]:	110.15
CAS:	1121-37-5

Physical Properties

Property code	Value	Unit	Source
affp	880.40	kJ/mol	NIST Webbook
basg	850.60	kJ/mol	NIST Webbook
gf	0.64	kJ/mol	Joback Method
hf	-154.79	kJ/mol	Joback Method
hfus	11.75	kJ/mol	Joback Method
hvap	37.75	kJ/mol	Joback Method
ie	9.10	eV	NIST Webbook
ie	9.28	eV	NIST Webbook
log10ws	-1.34		Crippen Method
logp	1.375		Crippen Method
mcvol	89.340	ml/mol	McGowan Method
pc	4072.51	kPa	Joback Method
tb	434.20	K	NIST Webbook
tc	634.97	K	Joback Method
tf	254.46	K	Joback Method
vc	0.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.24	J/mol×K	426.91	Joback Method
cpg	198.31	J/mol×K	461.59	Joback Method

cpg	211.38	J/mol×K	496.26	Joback Method
cpg	223.51	J/mol×K	530.94	Joback Method
cpg	234.78	J/mol×K	565.62	Joback Method
cpg	245.23	J/mol×K	600.29	Joback Method
cpg	254.95	J/mol×K	634.97	Joback Method
dvisc	0.0010953	Pa×s	254.46	Joback Method
dvisc	0.0010178	Pa×s	283.20	Joback Method
dvisc	0.0009586	Pa×s	311.94	Joback Method
dvisc	0.0009121	Pa×s	340.68	Joback Method
dvisc	0.0008745	Pa×s	369.43	Joback Method
dvisc	0.0008436	Pa×s	398.17	Joback Method
dvisc	0.0008178	Pa×s	426.91	Joback Method

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=C1121375&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
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
ie:	Ionization energy
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
tc:	Critical Temperature

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

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