

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	9.28	eV	NIST Webbook
ie	9.10	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.24	J/molxK	426.91	Joback Method
cpg	198.31	J/molxK	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	Paxs	254.46	Joback Method
dvisc	0.0010178	Paxs	283.20	Joback Method
dvisc	0.0009586	Paxs	311.94	Joback Method
dvisc	0.0009121	Paxs	340.68	Joback Method
dvisc	0.0008745	Paxs	369.43	Joback Method
dvisc	0.0008436	Paxs	398.17	Joback Method
dvisc	0.0008178	Paxs	426.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1121375&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

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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