Bicyclo[3.1.0]hexan-2-one, 5-(1-methylethyl)-

Other names:	Bicyclo[3.1.0]hexan-2-one, 5-isopropyl-
	Sabina ketone
	5-Isopropylbicyclo[3.1.0]hexan-2-one
	Sabine ketone
Inchi:	InChI=1S/C9H14O/c1-6(2)9-4-3-8(10)7(9)5-9/h6-7H,3-5H2,1-2H3
InchiKey:	MDDYCNAAAZKNAJ-UHFFFAOYSA-N
Formula:	C9H14O
SMILES:	CC(C)C12CCC(=O)C1C2
Mol. weight [g/mol]:	138.21
CAS:	513-20-2

Physical Properties

Property code	Value	Unit	Source
gf	15.88	kJ/mol	Joback Method
hf	-211.23	kJ/mol	Joback Method
hfus	5.02	kJ/mol	Joback Method
hvap	38.16	kJ/mol	Joback Method
log10ws	-1.93		Crippen Method
logp	2.012		Crippen Method
mcvol	117.520	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
rinpol	1156.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1179.00		NIST Webbook
rinpol	1154.00		NIST Webbook
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rinpol	1114.00	NIST Webbook
rinpol	1158.00	NIST Webbook
rinpol	1157.00	NIST Webbook
rinpol	1156.00	NIST Webbook
ripol	1651.00	NIST Webbook
ripol	1651.00	NIST Webbook
ripol	1606.00	NIST Webbook
ripol	1683.00	NIST Webbook
ripol	1675.00	NIST Webbook
ripol	1632.00	NIST Webbook
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ripol	1651.00		NIST Webbook
ripol	1651.00		NIST Webbook
ripol	1651.00		NIST Webbook
tb	486.42	K	Joback Method
tc	710.14	K	Joback Method
tf	304.19	K	Joback Method
vc	0.453	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.21	J/mol×K	486.42	Joback Method
cpg	294.86	J/mol×K	523.71	Joback Method
cpg	310.28	J/mol×K	560.99	Joback Method
cpg	324.61	J/mol×K	598.28	Joback Method
cpg	338.00	J/mol×K	635.57	Joback Method
cpg	350.60	J/mol×K	672.85	Joback Method
cpg	362.55	J/mol×K	710.14	Joback Method

Sources

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=C513202&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume