Bicyclo[3.1.0]hex-3-en-2-one, 5-(1-methylethyl)-

Other names: Dehydrosabinaketone
Dehydro sabinene ketone
Sabina ketone dehydro

Inchi: InChI=1S/C9H12O/c1-6(2)9-4-3-8(10)7(9)5-9/h3-4,6-7H,5H2,1-2H3

InchiKey: IBMZINAPWMATGM-UHFFFAOYSA-N

Formula: C9H12O

SMILES: CC(C)C12C=CC(=O)C1C2

Mol. weight [g/mol]: 136.19

CAS: 36262-12-1

Physical Properties

Property code	Value	Unit	Source
gf	45.84	kJ/mol	Joback Method
hf	-153.45	kJ/mol	Joback Method
hfus	6.25	kJ/mol	Joback Method
hvap	38.45	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	1.788		Crippen Method
mcvol	113.220	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
rinpol	1115.00		NIST Webbook
rinpol	1113.00		NIST Webbook
rinpol	1121.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1128.60		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1119.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1097.00		NIST Webbook
ripol	1643.00		NIST Webbook
ripol	1643.00		NIST Webbook

ripol	1643.00		NIST Webbook
ripol	1643.00		NIST Webbook
tb	485.58	K	Joback Method
tc	711.64	K	Joback Method
tf	304.95	K	Joback Method
vc	0.439	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.88	J/mol×K	485.58	Joback Method
cpg	277.23	J/mol×K	523.26	Joback Method
cpg	291.37	J/mol×K	560.93	Joback Method
cpg	304.45	J/mol×K	598.61	Joback Method
cpg	316.63	J/mol×K	636.29	Joback Method
cpg	328.06	J/mol×K	673.97	Joback Method
cpg	338.90	J/mol×K	711.64	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=C36262121&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