Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-trimethyl-, (1s)-

Other names: Levoverbenone
l-Verbenone
Verbenone, (L)-
2-Pinen-4-one, (1S,5S)-(-)-
(-)-Verbenone
(S)-(-)-Verbenone
S-Verbenone
(-)-cis-Verbenone
4,6,6-Trimethylbicyclo[3.1.1]hept-3-en-2-one, (1S,5S)-
NSC 6831
cis-Verbenone
pin-2-en-4-one

Inchi: InChI=1S/C10H14O/c1-6-4-9(11)8-5-7(6)10(8,2)3/h4,7-8H,5H2,1-3H3

InchiKey: DCSCXTJOXBUFGB-SFYZADRCSA-N

Formula: C10H14O

SMILES: CC1=CC(=O)C2CC1C2(C)C

Mol. weight [g/mol]: 150.22

Physical Properties

Property code	Value	Unit	Source
hfus	10.94	kJ/mol	Joback Method
hvap	58.35	kJ/mol	Cheméo Relay (1.0)
ie	9.27	eV	Cheméo Relay (1.0)
logp	2.178		Crippen Method
mcvol	127.310	ml/mol	McGowan Method
rinpol	1204.00		NIST Webbook
rinpol	1191.00		NIST Webbook
ripol	1723.00		NIST Webbook
tb	496.37	K	Cheméo Relay (1.0)
tf	355.52	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	307.39	J/mol×K	513.48	Joback Method
cpg	324.08	J/mol×K	551.25	Joback Method
cpg	339.67	J/mol×K	589.01	Joback Method
cpg	354.29	J/mol×K	626.78	Joback Method
cpg	368.08	J/mol×K	664.55	Joback Method
cpg	381.17	J/mol×K	702.31	Joback Method
cpg	393.70	J/mol×K	740.08	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1196016&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point