3-Carene, 2-acetyl-

Other names: 1-(4,7,7-Trimethylbicyclo[4.1.0]hept-4-enyl)ethanone (2-Acetylcarene)
Inchi: InChI=1S/C12H18O/c1-7-5-6-9-11(12(9,3)4)10(7)8(2)13/h5,9-11H,6H2,1-4H3
InchiKey: XCBVDXSSPNIVAO-UHFFFAOYSA-N
Formula: C12H18O
SMILES: CC(=O)C1C(C)=CCC2C1C2(C)C
Mol. weight [g/mol]: 178.27

Physical Properties

Property code	Value	Unit	Source
gf	30.06	kJ/mol	Joback Method
hf	-243.28	kJ/mol	Joback Method
hfus	19.28	kJ/mol	Joback Method
hvap	48.23	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.814		Crippen Method
mcvol	155.490	ml/mol	McGowan Method
pc	2445.89	kPa	Joback Method
ripol	1159.00		NIST Webbook
tb	540.62	K	Joback Method
tc	753.26	K	Joback Method
tf	335.99	K	Joback Method
vc	0.602	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.08	J/mol×K	540.62	Joback Method
cpg	411.05	J/mol×K	576.06	Joback Method
cpg	427.87	J/mol×K	611.50	Joback Method
cpg	443.66	J/mol×K	646.94	Joback Method
cpg	458.57	J/mol×K	682.38	Joback Method
cpg	472.74	J/mol×K	717.82	Joback Method
cpg	486.29	J/mol×K	753.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U156140&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume