(+)-3-Carene, 2-(acetylmethyl)-

Other names: +3-Carene-2-acetyle methyl
Inchi: InChI=1S/C13H20O/c1-8-5-6-11-12(13(11,3)4)10(8)7-9(2)14/h5,10-12H,6-7H2,1-4H3
InchiKey: MUMVVKJIYPHXLM-UHFFFAOYSA-N
Formula: C13H20O
SMILES: CC(=O)CC1C(C)=CCC2C1C2(C)C
Mol. weight [g/mol]: 192.30

Physical Properties

Property code	Value	Unit	Source
gf	38.48	kJ/mol	Joback Method
hf	-263.92	kJ/mol	Joback Method
hfus	21.87	kJ/mol	Joback Method
hvap	50.46	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	3.204		Crippen Method
mcvol	169.580	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
rinpol	1380.00		NIST Webbook
tb	563.50	K	Joback Method
tc	772.71	K	Joback Method
tf	347.26	K	Joback Method
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.30	J/mol×K	563.50	Joback Method
cpg	460.77	J/mol×K	598.37	Joback Method
cpg	478.13	J/mol×K	633.24	Joback Method
cpg	494.49	J/mol×K	668.11	Joback Method
cpg	510.01	J/mol×K	702.97	Joback Method
cpg	524.81	J/mol×K	737.84	Joback Method
cpg	539.02	J/mol×K	772.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U151802&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

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