Acetyl cedrene

Inchi: InChI=1S/C17H26O/c1-11-7-8-17-10-14(11)16(3,4)15(17)6-5-13(17)9-12(2)18/h9,11,14-1
InchiKey: WXETUDXXEZHSCS-OPFIGPJUSA-N
Formula: C17H26O
SMILES: CC(=O)C=C1CCC2C13CCC(C)C(C3)C2(C)C
Mol. weight [g/mol]: 246.39
CAS: 80449-58-7

Physical Properties

Property code	Value	Unit	Source
gf	140.45	kJ/mol	Joback Method
hf	-234.88	kJ/mol	Joback Method
hfus	21.46	kJ/mol	Joback Method
hvap	58.13	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.374		Crippen Method
mcvol	215.080	ml/mol	McGowan Method
pc	1900.26	kPa	Joback Method
rinpol	1770.10		NIST Webbook
rinpol	1768.00		NIST Webbook
ripol	2213.00		NIST Webbook
tb	668.77	K	Joback Method
tc	896.35	K	Joback Method
tf	427.74	K	Joback Method
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.83	J/mol×K	668.77	Joback Method
cpg	661.72	J/mol×K	706.70	Joback Method
cpg	682.64	J/mol×K	744.63	Joback Method
cpg	702.91	J/mol×K	782.56	Joback Method
cpg	722.85	J/mol×K	820.49	Joback Method
cpg	742.75	J/mol×K	858.42	Joback Method

cpg	762.95	J/mol×K	896.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80449587&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
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