Copabornyl acetate

Inchi: InChI=1S/C18H30O2/c1-11(2)13-6-8-17(4)15-7-9-18(17,5)16(14(15)10-13)20-12(3)19/h1
InchiKey: GJFAKHNOJIESPI-LJBIOTSSSA-N
Formula: C18H30O2
SMILES: CC(=O)OC1C2CC(C(C)C)CCC3(C)C2CCC13C
Mol. weight [g/mol]: 278.43

Physical Properties

Property code	Value	Unit	Source
gf	-11.74	kJ/mol	Joback Method
hf	-489.39	kJ/mol	Joback Method
hfus	22.46	kJ/mol	Joback Method
hvap	61.28	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	4.427		Crippen Method
mcvol	239.340	ml/mol	McGowan Method
pc	1651.11	kPa	Joback Method
rinpol	1661.00		NIST Webbook
ripol	1995.00		NIST Webbook
tb	702.32	K	Joback Method
tc	921.39	K	Joback Method
tf	431.64	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.32	J/mol×K	702.32	Joback Method
cpg	775.75	J/mol×K	738.83	Joback Method
cpg	798.31	J/mol×K	775.34	Joback Method
cpg	820.25	J/mol×K	811.86	Joback Method
cpg	841.85	J/mol×K	848.37	Joback Method
cpg	863.35	J/mol×K	884.88	Joback Method
cpg	885.01	J/mol×K	921.39	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R228967&Units=SI

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