8(15)-Cedren-9-«alpha»-ol, acetate

Inchi: InChI=1S/C17H26O2/c1-11-6-7-14-15(4,5)17(19-13(3)18)10-16(11,14)9-8-12(17)2/h11,1
InchiKey: YFYJISUDJNNDIJ-MDMQDRFWSA-N
Formula: C17H26O2
SMILES: C=C1CCC23CC1(OC(C)=O)C(C)(C)C2CCC3C
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	37.58	kJ/mol	Joback Method
hf	-343.65	kJ/mol	Joback Method
hfus	14.87	kJ/mol	Joback Method
hvap	58.76	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.101		Crippen Method
mcvol	220.950	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
rinpol	1729.00		NIST Webbook
rinpol	1729.00		NIST Webbook
tb	683.95	K	Joback Method
tc	912.08	K	Joback Method
tf	477.19	K	Joback Method
vc	0.843	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.97	J/mol×K	683.95	Joback Method
cpg	685.40	J/mol×K	721.97	Joback Method
cpg	706.28	J/mol×K	759.99	Joback Method
cpg	726.99	J/mol×K	798.01	Joback Method
cpg	747.92	J/mol×K	836.04	Joback Method
cpg	769.46	J/mol×K	874.06	Joback Method
cpg	792.00	J/mol×K	912.08	Joback Method

Sources

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=R129830&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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