

8(15)-Cedren-9-«alpha»-yl acetate

Other names:	Cedr-8(15)-en-9-«alpha»-ol, acetate
Inchi:	InChI=1S/C17H26O2/c1-10-6-7-15-16(4,5)13-8-17(10,15)9-14(11(13)2)19-12(3)18/h10,1
InchiKey:	UTZBRSREMTWJBB-GVUNGTEDSA-N
Formula:	C17H26O2
SMILES:	C=C1C(OC(C)=O)CC23CC1C(C)(C)C2CCC3C
Mol. weight [g/mol]:	262.39
CAS:	65082-66-8

Physical Properties

Property code	Value	Unit	Source
gf	35.36	kJ/mol	Joback Method
hf	-379.23	kJ/mol	Joback Method
hfus	22.24	kJ/mol	Joback Method
hvap	59.60	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.957		Crippen Method
mcvol	220.950	ml/mol	McGowan Method
pc	1804.63	kPa	Joback Method
rinpol	1729.00		NIST Webbook
rinpol	1723.00		NIST Webbook
rinpol	1729.00		NIST Webbook
rinpol	1743.00		NIST Webbook
tb	679.04	K	Joback Method
tc	899.33	K	Joback Method
tf	449.05	K	Joback Method
vc	0.844	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.85	J/mol×K	679.04	Joback Method
cpg	691.60	J/mol×K	715.75	Joback Method
cpg	712.47	J/mol×K	752.47	Joback Method
cpg	732.71	J/mol×K	789.18	Joback Method

cpg	752.57	J/mol×K	825.90	Joback Method
cpg	772.32	J/mol×K	862.61	Joback Method
cpg	792.19	J/mol×K	899.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65082668&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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