

1 «beta»-acetoxyfurano-3-eudesmene

Inchi:	InChI=1S/C17H24O3/c1-10-5-6-16(20-12(3)18)17(4)8-15-13(7-14(10)17)11(2)9-19-15/h5
InchiKey:	YXXLPOR TKKMOGV-PPRXNKMGS A-N
Formula:	C17H24O3
SMILES:	CC(=O)OC1CC=C(C)C2CC3C(C)=COC3CC12C
Mol. weight [g/mol]:	276.37

Physical Properties

Property code	Value	Unit	Source
gf	-74.18	kJ/mol	Joback Method
hf	-510.07	kJ/mol	Joback Method
hfus	34.07	kJ/mol	Joback Method
hvap	67.67	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.603		Crippen Method
mcvol	222.520	ml/mol	McGowan Method
pc	1887.08	kPa	Joback Method
ripol	2730.00		NIST Webbook
tb	728.08	K	Joback Method
tc	955.13	K	Joback Method
tf	461.80	K	Joback Method
vc	0.840	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.45	J/mol×K	728.08	Joback Method
cpg	710.11	J/mol×K	765.92	Joback Method
cpg	729.77	J/mol×K	803.76	Joback Method
cpg	748.57	J/mol×K	841.60	Joback Method
cpg	766.70	J/mol×K	879.45	Joback Method
cpg	784.29	J/mol×K	917.29	Joback Method
cpg	801.52	J/mol×K	955.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R395418&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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