

«gamma»-eudesmol acetate

Inchi:	InChI=1S/C17H28O2/c1-12-7-6-9-17(5)10-8-14(11-15(12)17)16(3,4)19-13(2)18/h14H,6-
InchiKey:	WJUQDFFDADGYQZ-YOEHRIQHSA-N
Formula:	C17H28O2
SMILES:	CC(=O)OC(C)(C)C1CCC2(C)CCCC(C)=C2C1
Mol. weight [g/mol]:	264.40

Physical Properties

Property code	Value	Unit	Source
gf	-60.51	kJ/mol	Joback Method
hf	-476.72	kJ/mol	Joback Method
hfus	17.18	kJ/mol	Joback Method
hvap	62.28	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.635		Crippen Method
mcvol	231.810	ml/mol	McGowan Method
pc	1774.35	kPa	Joback Method
rinpol	1782.00		NIST Webbook
rinpol	1780.00		NIST Webbook
rinpol	1768.00		NIST Webbook
rinpol	1778.00		NIST Webbook
rinpol	1778.00		NIST Webbook
rinpol	1768.00		NIST Webbook
ripol	2174.00		NIST Webbook
tb	701.34	K	Joback Method
tc	927.04	K	Joback Method
tf	427.43	K	Joback Method
vc	0.867	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.67	J/mol×K	701.34	Joback Method
cpg	713.43	J/mol×K	738.96	Joback Method
cpg	734.03	J/mol×K	776.57	Joback Method

cpg	753.66	J/mol×K	814.19	Joback Method
cpg	772.46	J/mol×K	851.81	Joback Method
cpg	790.63	J/mol×K	889.42	Joback Method
cpg	808.32	J/mol×K	927.04	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=R129776&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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