

«alpha»-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/h7,14-15
InchiKey:	DGEOCHVUGVJYQB-AYWPPYMVSA-N
Formula:	C17H28O2
SMILES:	CC(=O)OC(C)(C)C1CCC2(C)CCC=C(C)C2C1
Mol. weight [g/mol]:	264.40

Physical Properties

Property code	Value	Unit	Source
gf	-58.59	kJ/mol	Joback Method
hf	-485.59	kJ/mol	Joback Method
hfus	18.64	kJ/mol	Joback Method
hvap	61.30	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.491		Crippen Method
mcvol	231.810	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
rinpol	1779.00		NIST Webbook
rinpol	1748.00		NIST Webbook
rinpol	1779.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1748.00		NIST Webbook
rinpol	1795.00		NIST Webbook
rinpol	1785.00		NIST Webbook
tb	691.69	K	Joback Method
tc	916.62	K	Joback Method
tf	410.67	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.68	J/mol×K	691.69	Joback Method
cpg	716.12	J/mol×K	729.18	Joback Method
cpg	737.32	J/mol×K	766.67	Joback Method

cpg	757.44	J/mol×K	804.16	Joback Method
cpg	776.66	J/mol×K	841.65	Joback Method
cpg	795.13	J/mol×K	879.14	Joback Method
cpg	813.02	J/mol×K	916.62	Joback Method

Sources

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=R129741&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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