Kessanyl acetate

Inchi: InChI=1S/C17H28O3/c1-10-6-7-13-12(10)8-14-15(19-11(2)18)9-17(13,5)20-16(14,3)4/h1
InchiKey: CGBOQYJQRLRGIE-CBBLBBDDSA-N
Formula: C17H28O3
SMILES: CC(=O)OC1CC2(C)OC(C)(C)C1CC1C(C)CCC12
Mol. weight [g/mol]: 280.40

Physical Properties

Property code	Value	Unit	Source
gf	-123.65	kJ/mol	Joback Method
hf	-621.97	kJ/mol	Joback Method
hfus	30.35	kJ/mol	Joback Method
hvap	63.82	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.558		Crippen Method
mcvol	231.120	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	1827.00		NIST Webbook
rinpol	1806.70		NIST Webbook
rinpol	1856.00		NIST Webbook
ripol	2450.00		NIST Webbook
tb	706.43	K	Joback Method
tc	929.31	K	Joback Method
tf	454.18	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.75	J/mol×K	706.43	Joback Method
cpg	759.02	J/mol×K	743.58	Joback Method
cpg	781.42	J/mol×K	780.72	Joback Method
cpg	803.20	J/mol×K	817.87	Joback Method
cpg	824.60	J/mol×K	855.02	Joback Method
cpg	845.88	J/mol×K	892.17	Joback Method

cpg	867.29	J/mol×K	929.31	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=R2150&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume