Tau-Cadinol acetate

Inchi: InChI=1S/C17H28O2/c1-11(2)14-8-9-17(5,19-13(4)18)16-7-6-12(3)10-15(14)16/h10-11,1
InchiKey: TUKAHRUSXDHODN-UHFFFAOYSA-N
Formula: C17H28O2
SMILES: CC(=O)OC1(C)CCC(C(C)C)C2C=C(C)CCC21
Mol. weight [g/mol]: 264.40
CAS: 149197-48-8

Physical Properties

Property code	Value	Unit	Source
gf	-71.58	kJ/mol	Joback Method
hf	-502.46	kJ/mol	Joback Method
hfus	23.60	kJ/mol	Joback Method
hvap	61.90	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.347		Crippen Method
mcvol	231.810	ml/mol	McGowan Method
pc	1685.18	kPa	Joback Method
rinpol	1804.50		NIST Webbook
rinpol	1804.50		NIST Webbook
tb	689.81	K	Joback Method
tc	907.17	K	Joback Method
tf	389.01	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.83	J/mol×K	689.81	Joback Method
cpg	716.31	J/mol×K	726.04	Joback Method
cpg	737.62	J/mol×K	762.26	Joback Method
cpg	757.90	J/mol×K	798.49	Joback Method
cpg	777.26	J/mol×K	834.71	Joback Method
cpg	795.82	J/mol×K	870.94	Joback Method
cpg	813.71	J/mol×K	907.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C149197488&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume