7,7-dimethyl-2-methylenebicyclo[3.3.1]heptan-6-o acetate

Inchi: InChI=1S/C14H22O2/c1-9-5-6-11-7-12(9)8-14(3,4)13(11)16-10(2)15/h11-13H,1,5-8H2,2-

InchiKey: YHIVYSKPMIMKQJ-UHFFFAOYSA-N

Formula: C14H22O2

SMILES: C=C1CCC2CC1CC(C)(C)C2OC(C)=O

Mol. weight [g/mol]: 222.32

Physical Properties

Property code	Value	Unit	Source
gf	-49.55	kJ/mol	Joback Method
hf	-391.17	kJ/mol	Joback Method
hfus	19.46	kJ/mol	Joback Method
hvap	54.65	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.320		Crippen Method
mcvol	189.540	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
rinpol	1313.00		NIST Webbook
ripol	1646.00		NIST Webbook
tb	612.36	K	Joback Method
tc	828.67	K	Joback Method
tf	374.12	K	Joback Method
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.15	J/mol×K	612.36	Joback Method
cpg	544.62	J/mol×K	648.41	Joback Method
cpg	563.96	J/mol×K	684.46	Joback Method
cpg	582.28	J/mol×K	720.52	Joback Method
cpg	599.71	J/mol×K	756.57	Joback Method
cpg	616.35	J/mol×K	792.62	Joback Method
cpg	632.32	J/mol×K	828.67	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R344539&Units=SI

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