7-Acetyl-2,2,6-trimethylbicyclo[4.2.0]octane

Inchi: InChI=1S/C13H22O2/c1-9(14)15-11-8-10-12(2,3)6-5-7-13(10,11)4/h10-11H,5-8H2,1-4H3
InchiKey: SAWHMFWVBIJWKO-UHFFFAOYSA-N
Formula: C13H22O2
SMILES: CC(=O)OC1CC2C(C)(C)CCCC12C
Mol. weight [g/mol]: 210.31

Physical Properties

Property code	Value	Unit	Source
gf	-104.44	kJ/mol	Joback Method
hf	-433.37	kJ/mol	Joback Method
hfus	13.83	kJ/mol	Joback Method
hvap	50.94	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.154		Crippen Method
mcvol	179.750	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
rinpol	1370.00		NIST Webbook
rinpol	1370.00		NIST Webbook
ripol	1763.00		NIST Webbook
ripol	1763.00		NIST Webbook
tb	586.29	K	Joback Method
tc	805.67	K	Joback Method
tf	376.59	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.76	J/mol×K	586.29	Joback Method
cpg	509.83	J/mol×K	622.85	Joback Method
cpg	528.72	J/mol×K	659.42	Joback Method
cpg	546.65	J/mol×K	695.98	Joback Method
cpg	563.86	J/mol×K	732.54	Joback Method
cpg	580.56	J/mol×K	769.11	Joback Method

cpg	596.98	J/mol×K	805.67	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=R228912&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