3,3-dimethylcyclohex-6-en-1-yl acetate

Inchi: InChI=1S/C10H16O2/c1-8(11)12-9-5-4-6-10(2,3)7-9/h5H,4,6-7H2,1-3H3
InchiKey: ZCVJWHUHIYWLMG-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: CC(=O)OC1=CCCC(C)(C)C1
Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	-161.31	kJ/mol	Joback Method
hf	-378.66	kJ/mol	Joback Method
hfus	10.81	kJ/mol	Joback Method
hvap	47.24	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.643		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
rinpol	1158.00		NIST Webbook
rinpol	1158.00		NIST Webbook
tb	528.42	K	Joback Method
tc	745.55	K	Joback Method
tf	319.18	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.44	J/mol×K	528.42	Joback Method
cpg	353.63	J/mol×K	564.61	Joback Method
cpg	368.87	J/mol×K	600.80	Joback Method
cpg	383.24	J/mol×K	636.99	Joback Method
cpg	396.86	J/mol×K	673.18	Joback Method
cpg	409.80	J/mol×K	709.36	Joback Method
cpg	422.17	J/mol×K	745.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R216330&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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