2-(2,2-dimethyl-6-methylenecyclohexyl)-ethyl acetate

Inchi: InChI=1S/C13H22O2/c1-10-6-5-8-13(3,4)12(10)7-9-15-11(2)14/h12H,1,5-9H2,2-4H3
InchiKey: JCSFOVFIEQAJIG-UHFFFAOYSA-N
Formula: C13H22O2
SMILES: C=C1CCCC(C)(C)C1CCOC(C)=O
Mol. weight [g/mol]: 210.31

Physical Properties

Property code	Value	Unit	Source
gf	-111.01	kJ/mol	Joback Method
hf	-422.99	kJ/mol	Joback Method
hfus	17.66	kJ/mol	Joback Method
hvap	52.82	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	3.322		Crippen Method
mcvol	186.310	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
ripol	1813.00		NIST Webbook
ripol	1813.00		NIST Webbook
tb	587.41	K	Joback Method
tc	792.89	K	Joback Method
tf	349.15	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.41	J/mol×K	587.41	Joback Method
cpg	503.14	J/mol×K	621.66	Joback Method
cpg	520.92	J/mol×K	655.90	Joback Method
cpg	537.83	J/mol×K	690.15	Joback Method
cpg	553.95	J/mol×K	724.39	Joback Method
cpg	569.37	J/mol×K	758.64	Joback Method
cpg	584.15	J/mol×K	792.89	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=R344084&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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