2-(2,2-dimethyl-6-methylenecyclohexyl)-acetaldeh

Inchi: InChI=1S/C11H18O/c1-9-5-4-7-11(2,3)10(9)6-8-12/h8,10H,1,4-7H2,2-3H3
InchiKey: WJGGZGYLEUUXHR-UHFFFAOYSA-N
Formula: C11H18O
SMILES: C=C1CCCC(C)(C)C1CC=O
Mol. weight [g/mol]: 166.26

Physical Properties

Property code	Value	Unit	Source
gf	6.55	kJ/mol	Joback Method
hf	-222.49	kJ/mol	Joback Method
hfus	11.98	kJ/mol	Joback Method
hvap	45.93	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.958		Crippen Method
mcvol	152.260	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
ripol	1662.00		NIST Webbook
tb	514.02	K	Joback Method
tc	723.10	K	Joback Method
tf	296.45	K	Joback Method
vc	0.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.65	J/mol×K	514.02	Joback Method
cpg	376.31	J/mol×K	548.87	Joback Method
cpg	392.93	J/mol×K	583.71	Joback Method
cpg	408.60	J/mol×K	618.56	Joback Method
cpg	423.43	J/mol×K	653.41	Joback Method
cpg	437.50	J/mol×K	688.25	Joback Method
cpg	450.90	J/mol×K	723.10	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=R344064&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