2,3,3-Trimethyl-3-cyclopentene acetaldehyde

Inchi: InChI=1S/C9H16O/c1-7-8(6-10)4-5-9(7,2)3/h6-8H,4-5H2,1-3H3
InchiKey: SPHPESDVRLMLFF-UHFFFAOYSA-N
Formula: C9H16O
SMILES: CC1C(C=O)CCC1(C)C
Mol. weight [g/mol]: 140.22

Physical Properties

Property code	Value	Unit	Source
gf	-58.98	kJ/mol	Joback Method
hf	-279.63	kJ/mol	Joback Method
hfus	11.13	kJ/mol	Joback Method
hvap	40.84	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	2.258		Crippen Method
mcvol	128.380	ml/mol	McGowan Method
pc	2925.00	kPa	Joback Method
rinpol	1117.00		NIST Webbook
tb	460.16	K	Joback Method
tc	665.26	K	Joback Method
tf	259.51	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.61	J/mol×K	460.16	Joback Method
cpg	301.64	J/mol×K	494.34	Joback Method
cpg	317.61	J/mol×K	528.53	Joback Method
cpg	332.61	J/mol×K	562.71	Joback Method
cpg	346.74	J/mol×K	596.89	Joback Method
cpg	360.08	J/mol×K	631.07	Joback Method
cpg	372.72	J/mol×K	665.26	Joback Method

Sources

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=R419326&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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