2,2,3-Trimethyl-3-cyclopentene-1-acetaldehyde

Inchi: InChI=1S/C9H14O/c1-7-4-5-8(6-10)9(7,2)3/h4,6,8H,5H2,1-3H3
InchiKey: KUSHNIVDXXIKCE-UHFFFAOYSA-N
Formula: C9H14O
SMILES: CC1=CCC(C=O)C1(C)C
Mol. weight [g/mol]: 138.21

Physical Properties

Property code	Value	Unit	Source
gf	-30.94	kJ/mol	Joback Method
hf	-212.98	kJ/mol	Joback Method
hfus	10.90	kJ/mol	Joback Method
hvap	42.10	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	2.178		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
rinpol	1097.00		NIST Webbook
rinpol	1097.00		NIST Webbook
tb	468.97	K	Joback Method
tc	677.79	K	Joback Method
tf	277.03	K	Joback Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.64	J/mol×K	468.97	Joback Method
cpg	284.59	J/mol×K	503.77	Joback Method
cpg	298.56	J/mol×K	538.58	Joback Method
cpg	311.64	J/mol×K	573.38	Joback Method
cpg	323.94	J/mol×K	608.18	Joback Method
cpg	335.54	J/mol×K	642.98	Joback Method
cpg	346.54	J/mol×K	677.79	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=R288261&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