Cyclohexene-1-acetaldehyde, 2,6,6-trimethyl

Inchi: InChI=1S/C10H18O/c1-8-5-4-6-10(2,3)9(8)7-11/h7-9H,4-6H2,1-3H3
InchiKey: MPLGIGIOVUTMJA-UHFFFAOYSA-N
Formula: C10H18O
SMILES: CC1CCCC(C)(C)C1C=O
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
gf	-62.66	kJ/mol	Joback Method
hf	-306.43	kJ/mol	Joback Method
hfus	11.62	kJ/mol	Joback Method
hvap	43.23	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.648		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2712.67	kPa	Joback Method
rinpol	1238.00		NIST Webbook
tb	487.31	K	Joback Method
tc	697.48	K	Joback Method
tf	267.26	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.83	J/mol×K	487.31	Joback Method
cpg	348.62	J/mol×K	522.34	Joback Method
cpg	366.29	J/mol×K	557.37	Joback Method
cpg	382.94	J/mol×K	592.39	Joback Method
cpg	398.65	J/mol×K	627.42	Joback Method
cpg	413.51	J/mol×K	662.45	Joback Method
cpg	427.62	J/mol×K	697.48	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=R199656&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume