1-Cyclohexene-1-carboxaldehyde, 2,6,6-trimethyl-

Other names: «beta»-Cyclocitral
1-Formyl-2,6,6-trimethyl-1-cyclohexene
2,6,6-trimethyl-cyclohexene-1-carboxaldehyde
2,6,6-Trimethyl-1-cyclohexene-1-carboxaldehyde
2,6,6-trimethylcyclohexene-1-carbaldehyde

Inchi: InChI=1S/C10H16O/c1-8-5-4-6-10(2,3)9(8)7-11/h7H,4-6H2,1-3H3

InchiKey: MOQGCGNUWBPGTQ-UHFFFAOYSA-N

Formula: C10H16O

SMILES: CC1=C(C=O)C(C)(C)CCC1

Mol. weight [g/mol]: 152.23

CAS: 432-25-7

Physical Properties

Property code	Value	Unit	Source
gf	-36.54	kJ/mol	Joback Method
hf	-230.91	kJ/mol	Joback Method
hfus	9.93	kJ/mol	Joback Method
hvap	45.47	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.712		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
rinpol	1196.00		NIST Webbook
rinpol	1196.00		NIST Webbook
rinpol	1190.00		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1200.00		NIST Webbook
rinpol	1200.00		NIST Webbook
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rinpol	1194.00		NIST Webbook
rinpol	1197.00		NIST Webbook
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ripol	1635.00		NIST Webbook
ripol	1593.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1638.00		NIST Webbook
tb	505.77	K	Joback Method
tc	720.94	K	Joback Method
tf	301.54	K	Joback Method

vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.28	J/mol×K	505.77	Joback Method
cpg	329.19	J/mol×K	541.63	Joback Method
cpg	344.11	J/mol×K	577.49	Joback Method
cpg	358.15	J/mol×K	613.35	Joback Method
cpg	371.41	J/mol×K	649.21	Joback Method
cpg	383.99	J/mol×K	685.08	Joback Method
cpg	396.00	J/mol×K	720.94	Joback Method

Sources

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=C432257&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume