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

Other names: 2,6,6-Trimethyl-2-cyclohexene-1-carboxaldehyde
«alpha»-Cyclocitral
Filipendulal
1-Formyl-2,6,6-trimethyl-2-cyclohexene
2,6,6-Trimethylcyclohex-2-en-1-carboxaldehyde
2,6,6-trimethylcyclohex-2-ene-1-carbaldehyde

Inchi: InChI=1S/C10H16O/c1-8-5-4-6-10(2,3)9(8)7-11/h5,7,9H,4,6H2,1-3H3

InchiKey: ZVZRJSHOOULAGB-UHFFFAOYSA-N

Formula: C10H16O

SMILES: CC1=CCCC(C)(C)C1C=O

Mol. weight [g/mol]: 152.23

CAS: 432-24-6

Physical Properties

Property code	Value	Unit	Source
gf	-34.62	kJ/mol	Joback Method
hf	-239.78	kJ/mol	Joback Method
hfus	11.39	kJ/mol	Joback Method
hvap	44.50	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.568		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
rinpol	1102.00		NIST Webbook
rinpol	1097.50		NIST Webbook
rinpol	1122.90		NIST Webbook
rinpol	1102.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1096.30		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1124.00		NIST Webbook

ripol	1420.00		NIST Webbook
ripol	1430.00		NIST Webbook
ripol	1420.00		NIST Webbook
tb	496.12	K	Joback Method
tc	709.88	K	Joback Method
tf	284.78	K	Joback Method
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.56	J/mol×K	496.12	Joback Method
cpg	330.31	J/mol×K	531.75	Joback Method
cpg	346.01	J/mol×K	567.37	Joback Method
cpg	360.76	J/mol×K	603.00	Joback Method
cpg	374.68	J/mol×K	638.62	Joback Method
cpg	387.85	J/mol×K	674.25	Joback Method
cpg	400.37	J/mol×K	709.88	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=C432246&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume