1,3-Cyclohexadiene-1-carboxaldehyde, 2,6,6-trimethyl-

Other names: Safranal
2,6,6-Trimethyl-1,3-cyclohexadiene-1-carboxaldehyde
2,3-dihydro-2,2,6-trimethylbenzaldehyde
Inchi: InChI=1S/C10H14O/c1-8-5-4-6-10(2,3)9(8)7-11/h4-5,7H,6H2,1-3H3
InchiKey: SGAWOGXMMPSZPB-UHFFFAOYSA-N
Formula: C10H14O
SMILES: CC1=C(C=O)C(C)(C)CC=C1
Mol. weight [g/mol]: 150.22
CAS: 116-26-7

Physical Properties

Property code	Value	Unit	Source
gf	-6.58	kJ/mol	Joback Method
hf	-173.13	kJ/mol	Joback Method
hfus	11.15	kJ/mol	Joback Method
hvap	45.76	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.488		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinpol	1173.00		NIST Webbook
rinpol	1207.60		NIST Webbook
rinpol	1189.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1201.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1197.00		NIST Webbook
rinpol	1198.00		NIST Webbook
rinpol	1214.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1201.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1197.00		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	1205.00		NIST Webbook

rinpol	1201.00	NIST Webbook
rinpol	1201.00	NIST Webbook
rinpol	1192.00	NIST Webbook
rinpol	1201.00	NIST Webbook
rinpol	1201.00	NIST Webbook
rinpol	1202.00	NIST Webbook
rinpol	1181.00	NIST Webbook
rinpol	1181.00	NIST Webbook
rinpol	1207.60	NIST Webbook
rinpol	1218.00	NIST Webbook
rinpol	1199.00	NIST Webbook
rinpol	1196.00	NIST Webbook
rinpol	1201.00	NIST Webbook
rinpol	1205.00	NIST Webbook
rinpol	1203.00	NIST Webbook
rinpol	1214.00	NIST Webbook
rinpol	1180.00	NIST Webbook
rinpol	1197.00	NIST Webbook
rinpol	1189.00	NIST Webbook
rinpol	1198.00	NIST Webbook
rinpol	1201.00	NIST Webbook
rinpol	1189.00	NIST Webbook
rinpol	1175.00	NIST Webbook
rinpol	1201.00	NIST Webbook
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rinpol	1198.00	NIST Webbook
rinpol	1172.00	NIST Webbook
rinpol	1207.00	NIST Webbook
rinpol	1177.00	NIST Webbook
rinpol	1212.00	NIST Webbook
rinpol	1173.00	NIST Webbook
rinpol	1171.00	NIST Webbook
rinpol	1189.00	NIST Webbook
rinpol	1203.00	NIST Webbook
rinpol	1201.00	NIST Webbook
rinpol	1207.00	NIST Webbook
rinpol	1196.00	NIST Webbook
rinpol	1174.00	NIST Webbook
rinpol	1197.00	NIST Webbook
rinpol	1167.00	NIST Webbook
ripol	1597.00	NIST Webbook
ripol	1596.00	NIST Webbook
ripol	1648.00	NIST Webbook
ripol	1642.00	NIST Webbook

ripol	1622.00		NIST Webbook
ripol	1596.00		NIST Webbook
ripol	1596.00		NIST Webbook
ripol	1596.00		NIST Webbook
ripol	1614.00		NIST Webbook
ripol	1617.00		NIST Webbook
ripol	1617.00		NIST Webbook
ripol	1648.00		NIST Webbook
tb	504.93	K	Joback Method
tc	722.27	K	Joback Method
tf	302.30	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.18	J/mol×K	504.93	Joback Method
cpg	310.85	J/mol×K	541.15	Joback Method
cpg	324.56	J/mol×K	577.38	Joback Method
cpg	337.42	J/mol×K	613.60	Joback Method
cpg	349.54	J/mol×K	649.82	Joback Method
cpg	361.03	J/mol×K	686.05	Joback Method
cpg	371.98	J/mol×K	722.27	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=C116267&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

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https://www.chemeo.com/cid/67-764-0/1-3-Cyclohexadiene-1-carboxaldehyde-2-6-6-trimethyl.pdf
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