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

Other names: 2,6,6-Trimethyl-1-cyclohexene-1-acetaldehyde
«beta»-Cyclo-homocitral
«beta»-Homocyclocitral

Inchi: InChI=1S/C11H18O/c1-9-5-4-7-11(2,3)10(9)6-8-12/h8H,4-7H2,1-3H3

InchiKey: VHTFHZGAMYUZEP-UHFFFAOYSA-N

Formula: C11H18O

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

Mol. weight [g/mol]: 166.26

CAS: 472-66-2

Physical Properties

Property code	Value	Unit	Source
gf	-28.12	kJ/mol	Joback Method
hf	-251.55	kJ/mol	Joback Method
hfus	12.52	kJ/mol	Joback Method
hvap	47.69	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	3.102		Crippen Method
mcvol	152.260	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
rinpol	1235.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1254.00		NIST Webbook
rinpol	1257.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1254.00		NIST Webbook
rinpol	1261.30		NIST Webbook
rinpol	1237.30		NIST Webbook
rinpol	1236.00		NIST Webbook
tb	528.65	K	Joback Method
tc	740.38	K	Joback Method
tf	312.81	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.42	J/mol×K	528.65	Joback Method
cpg	376.08	J/mol×K	563.94	Joback Method
cpg	391.76	J/mol×K	599.23	Joback Method
cpg	406.57	J/mol×K	634.52	Joback Method
cpg	420.60	J/mol×K	669.81	Joback Method
cpg	433.96	J/mol×K	705.09	Joback Method
cpg	446.74	J/mol×K	740.38	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	331.70	K	0.05	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C472662&Units=SI
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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume