Acetaldehyde, (3,3-dimethylcyclohexylidene)-, (Z)-

Other names: «delta»1,«alpha»-Cyclohexaneacetaldehyde, 3,3-dimethyl-, (Z)-
(Z)-3,3-Dimethyl-«delta»1,«alpha»-cyclohexaneacetaldehyde
(Z)-3,3-Dimethylcyclohexane-«delta»1,«alpha»-acetaldehyde
cis-3,3-Dimethyl-«delta»1,«alpha»-Cyclohexanacetaldehyde
cis-3,3-Dimethyl-«delta»1,«alpha»-Cyclohexaneacetaldehyde
cis-3,3-Dimethylcyclohexylideneethanal
(2Z)-(3,3-Dimethylcyclohexylidene)ethanal
Acetaldehyde, (3,3-dimethylcyclohexylidene)-, (2Z)-
Acetaldehyde, 2-(3,3-dimethylcyclohexylidene)-, (2Z)-
Grandlure III

Inchi: InChI=1S/C10H16O/c1-10(2)6-3-4-9(8-10)5-7-11/h5,7H,3-4,6,8H2,1-2H3/b9-5-

InchiKey: TYHKWUGMKWVPDI-UITAMQMPSA-N

Formula: C10H16O

SMILES: CC1(C)CCCC(=CC=O)C1

Mol. weight [g/mol]: 152.23

CAS: 26532-24-1

Physical Properties

Property code	Value	Unit	Source
gf	-1.78	kJ/mol	Joback Method
hf	-189.72	kJ/mol	Joback Method
hfus	9.80	kJ/mol	Joback Method
hvap	44.64	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.712		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
ripol	1799.00		NIST Webbook
tb	503.29	K	Joback Method
tc	721.27	K	Joback Method
tf	286.10	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.64	J/mol×K	503.29	Joback Method
cpg	329.38	J/mol×K	539.62	Joback Method
cpg	344.99	J/mol×K	575.95	Joback Method
cpg	359.60	J/mol×K	612.28	Joback Method
cpg	373.32	J/mol×K	648.61	Joback Method
cpg	386.28	J/mol×K	684.94	Joback Method
cpg	398.60	J/mol×K	721.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26532241&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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