

(1,2,2-trimethyl-3-cyclopenten-1-yl)acetaldehyde

Inchi:	InChI=1S/C10H16O/c1-9(2)5-4-6-10(9,3)7-8-11/h4-5,8H,6-7H2,1-3H3
InchiKey:	AIZSHOZHOLKAGD-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	CC1(C)C=CCC1(C)CC=O
Mol. weight [g/mol]:	152.23

Physical Properties

Property code	Value	Unit	Source
gf	-18.38	kJ/mol	Joback Method
hf	-206.91	kJ/mol	Joback Method
hfus	7.58	kJ/mol	Joback Method
hvap	42.51	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.568		Crippen Method
mvol	138.170	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
ripol	1472.00		NIST Webbook
ripol	1472.00		NIST Webbook
tb	487.11	K	Joback Method
tc	700.59	K	Joback Method
tf	299.68	K	Joback Method
vc	0.534	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.32	J/mol×K	487.11	Joback Method
cpg	329.55	J/mol×K	522.69	Joback Method
cpg	344.49	J/mol×K	558.27	Joback Method
cpg	358.32	J/mol×K	593.85	Joback Method
cpg	371.25	J/mol×K	629.43	Joback Method
cpg	383.45	J/mol×K	665.01	Joback Method
cpg	395.13	J/mol×K	700.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U365943&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	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
ripl:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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