3,3-dimethylcyclohex-6-eneacetaldehyde

Inchi: InChI=1S/C10H16O/c1-10(2)6-3-4-9(8-10)5-7-11/h4,7H,3,5-6,8H2,1-2H3
InchiKey: WHHNLCPUSNYEJH-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CC1(C)CCC=C(CC=O)C1
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	-26.91	kJ/mol	Joback Method
hf	-219.44	kJ/mol	Joback Method
hfus	10.31	kJ/mol	Joback Method
hvap	44.81	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.712		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2976.29	kPa	Joback Method
rinpol	1125.00		NIST Webbook
tb	500.79	K	Joback Method
tc	714.74	K	Joback Method
tf	289.02	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.79	J/mol×K	500.79	Joback Method
cpg	329.11	J/mol×K	536.45	Joback Method
cpg	344.38	J/mol×K	572.11	Joback Method
cpg	358.69	J/mol×K	607.76	Joback Method
cpg	372.17	J/mol×K	643.42	Joback Method
cpg	384.91	J/mol×K	679.08	Joback Method
cpg	397.02	J/mol×K	714.74	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=R216350&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume