3,3-dimethylcyclohex-6-enecarboxaldehyde

Inchi: InChI=1S/C9H14O/c1-9(2)5-3-4-8(6-9)7-10/h4,7H,3,5-6H2,1-2H3
InchiKey: BVHNHGGBDBZFPW-UHFFFAOYSA-N
Formula: C9H14O
SMILES: CC1(C)CCC=C(C=O)C1
Mol. weight [g/mol]: 138.21

Physical Properties

Property code	Value	Unit	Source
gf	-35.33	kJ/mol	Joback Method
hf	-198.80	kJ/mol	Joback Method
hfus	7.73	kJ/mol	Joback Method
hvap	42.58	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.322		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
rinpol	1152.00		NIST Webbook
tb	477.91	K	Joback Method
tc	695.22	K	Joback Method
tf	277.75	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.35	J/mol×K	477.91	Joback Method
cpg	283.86	J/mol×K	514.13	Joback Method
cpg	298.30	J/mol×K	550.35	Joback Method
cpg	311.79	J/mol×K	586.57	Joback Method
cpg	324.44	J/mol×K	622.78	Joback Method
cpg	336.34	J/mol×K	659.00	Joback Method
cpg	347.62	J/mol×K	695.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R216365&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume