3,3-dimethylcyclohexaneacetaldehyde

Inchi: InChI=1S/C10H18O/c1-10(2)6-3-4-9(8-10)5-7-11/h7,9H,3-6,8H2,1-2H3
InchiKey: BDNFKTJPCKWKHE-UHFFFAOYSA-N
Formula: C10H18O
SMILES: CC1(C)CCCC(CC=O)C1
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
gf	-54.95	kJ/mol	Joback Method
hf	-286.09	kJ/mol	Joback Method
hfus	10.55	kJ/mol	Joback Method
hvap	43.54	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.792		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2808.38	kPa	Joback Method
rinpol	1130.00		NIST Webbook
tb	491.98	K	Joback Method
tc	702.37	K	Joback Method
tf	271.50	K	Joback Method
vc	0.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.44	J/mol×K	491.98	Joback Method
cpg	347.82	J/mol×K	527.04	Joback Method
cpg	365.06	J/mol×K	562.11	Joback Method
cpg	381.26	J/mol×K	597.17	Joback Method
cpg	396.52	J/mol×K	632.24	Joback Method
cpg	410.95	J/mol×K	667.30	Joback Method
cpg	424.64	J/mol×K	702.37	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=R216370&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