2- hydroxy-2,6,6-trimethylcyclo-hexane-1-carboxaldehyde

Inchi: InChI=1S/C10H18O2/c1-9(2)5-4-6-10(3,12)8(9)7-11/h7-8,12H,4-6H2,1-3H3
InchiKey: HRPCKEAUAIGZEF-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: CC1(C)CCCC(C)(O)C1C=O
Mol. weight [g/mol]: 170.25

Physical Properties

Property code	Value	Unit	Source
gf	-204.97	kJ/mol	Joback Method
hf	-443.42	kJ/mol	Joback Method
hfus	9.41	kJ/mol	Joback Method
hvap	58.76	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	1.763		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	3145.56	kPa	Joback Method
ripol	1860.00		NIST Webbook
ripol	1860.00		NIST Webbook
tb	579.73	K	Joback Method
tc	783.69	K	Joback Method
tf	351.98	K	Joback Method
vc	0.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.02	J/mol×K	579.73	Joback Method
cpg	407.02	J/mol×K	613.72	Joback Method
cpg	421.19	J/mol×K	647.72	Joback Method
cpg	434.70	J/mol×K	681.71	Joback Method
cpg	447.70	J/mol×K	715.70	Joback Method
cpg	460.35	J/mol×K	749.70	Joback Method
cpg	472.80	J/mol×K	783.69	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=R315878&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume