4-Hydroxy-2,6,6-trimethylcyclohex-1-enecarbalde

Inchi: InChI=1S/C10H16O2/c1-7-4-8(12)5-10(2,3)9(7)6-11/h6,8,12H,4-5H2,1-3H3
InchiKey: SWPMTVXRLXPNDP-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: CC1=C(C=O)C(C)(C)CC(O)C1
Mol. weight [g/mol]: 168.23
CAS: 35692-94-5

Physical Properties

Property code	Value	Unit	Source
gf	-181.07	kJ/mol	Joback Method
hf	-403.48	kJ/mol	Joback Method
hfus	15.08	kJ/mol	Joback Method
hvap	61.84	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	1.683		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	3124.49	kPa	Joback Method
rinpol	1431.00		NIST Webbook
tb	593.28	K	Joback Method
tc	793.65	K	Joback Method
tf	358.12	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.03	J/mol×K	593.28	Joback Method
cpg	384.38	J/mol×K	626.68	Joback Method
cpg	397.07	J/mol×K	660.07	Joback Method
cpg	409.17	J/mol×K	693.47	Joback Method
cpg	420.76	J/mol×K	726.86	Joback Method
cpg	431.91	J/mol×K	760.26	Joback Method
cpg	442.72	J/mol×K	793.65	Joback Method

Sources

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=C35692945&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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