2,4,4-Trimethyl-3-carboxaldehyde-5-hydroxy-2,5-c

Inchi: InChI=1S/C10H12O3/c1-6-7(5-11)10(2,3)9(13)4-8(6)12/h4-5,13H,1-3H3
InchiKey: YZSYPUKZYXIWGT-UHFFFAOYSA-N
Formula: C10H12O3
SMILES: CC1=C(C=O)C(C)(C)C(O)=CC1=O
Mol. weight [g/mol]: 180.20

Physical Properties

Property code	Value	Unit	Source
gf	-275.62	kJ/mol	Joback Method
hf	-474.53	kJ/mol	Joback Method
hfus	14.36	kJ/mol	Joback Method
hvap	67.35	kJ/mol	Joback Method
log10ws	-1.75		Crippen Method
logp	1.553		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
rinpol	1329.00		NIST Webbook
rinpol	1329.00		NIST Webbook
tb	669.91	K	Joback Method
tc	884.92	K	Joback Method
tf	443.86	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.61	J/mol×K	669.91	Joback Method
cpg	381.04	J/mol×K	705.75	Joback Method
cpg	392.04	J/mol×K	741.58	Joback Method
cpg	402.67	J/mol×K	777.42	Joback Method
cpg	412.99	J/mol×K	813.25	Joback Method
cpg	423.08	J/mol×K	849.09	Joback Method
cpg	433.00	J/mol×K	884.92	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R590668&Units=SI

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