4-Hydroxy-2,6,6-trimethyl-1-cyclohexene-1-carbox

Inchi: InChI=1S/C11H18O/c1-5-10-8(2)6-9(12)7-11(10,3)4/h5,9,12H,1,6-7H2,2-4H3
InchiKey: JBNNEBXFMFDBSS-UHFFFAOYSA-N
Formula: C11H18O
SMILES: C=CC1=C(C)CC(O)CC1(C)C
Mol. weight [g/mol]: 166.26

Physical Properties

Property code	Value	Unit	Source
gf	14.71	kJ/mol	Joback Method
hf	-213.11	kJ/mol	Joback Method
hfus	14.11	kJ/mol	Joback Method
hvap	56.67	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.670		Crippen Method
mcvol	152.260	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
rinpol	1344.00		NIST Webbook
rinpol	1344.00		NIST Webbook
tb	564.18	K	Joback Method
tc	762.27	K	Joback Method
tf	325.63	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.00	J/mol×K	564.18	Joback Method
cpg	393.97	J/mol×K	597.19	Joback Method
cpg	408.17	J/mol×K	630.21	Joback Method
cpg	421.67	J/mol×K	663.22	Joback Method
cpg	434.55	J/mol×K	696.24	Joback Method
cpg	446.90	J/mol×K	729.25	Joback Method
cpg	458.81	J/mol×K	762.27	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=R590702&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