4-hydroxy-4-(3«xi»-hydroxy-1-butenyl)-3,5,5-trime

Other names: 2-Cyclohexen-1-one-4-ol, 3,5,5-trimethyl, 4-(3-hydroxy-1-butenyl)
Inchi: InChI=1S/C13H20O3/c1-9-7-11(15)8-12(3,4)13(9,16)6-5-10(2)14/h5-7,10,14,16H,8H2,1-
InchiKey: KPQMCAKZRXOZLB-AATRIKPKSA-N
Formula: C13H20O3
SMILES: CC1=CC(=O)CC(C)(C)C1(O)C=CC(C)O
Mol. weight [g/mol]: 224.30

Physical Properties

Property code	Value	Unit	Source
gf	-233.78	kJ/mol	Joback Method
hf	-531.10	kJ/mol	Joback Method
hfus	14.93	kJ/mol	Joback Method
hvap	80.48	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	1.600		Crippen Method
mcvol	187.880	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
rinpol	1768.00		NIST Webbook
tb	772.24	K	Joback Method
tc	978.61	K	Joback Method
tf	470.27	K	Joback Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.30	J/mol×K	772.24	Joback Method
cpg	582.00	J/mol×K	806.64	Joback Method
cpg	596.66	J/mol×K	841.03	Joback Method
cpg	611.44	J/mol×K	875.43	Joback Method
cpg	626.50	J/mol×K	909.82	Joback Method
cpg	642.00	J/mol×K	944.22	Joback Method
cpg	658.11	J/mol×K	978.61	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=R194993&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