2-Isopropylidene-3-methyl-cyclopent-2-en-4-ol

Inchi: InChI=1S/C9H14O/c1-6(2)8-4-5-9(10)7(8)3/h9-10H,1,4-5H2,2-3H3
InchiKey: KRQBZXULJLUYMI-UHFFFAOYSA-N
Formula: C9H14O
SMILES: C=C(C)C1=C(C)C(O)CC1
Mol. weight [g/mol]: 138.21

Physical Properties

Property code	Value	Unit	Source
gf	14.62	kJ/mol	Joback Method
hf	-170.36	kJ/mol	Joback Method
hfus	14.94	kJ/mol	Joback Method
hvap	53.59	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.034		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	3239.34	kPa	Joback Method
rinpol	1220.00		NIST Webbook
rinpol	1220.00		NIST Webbook
tb	518.46	K	Joback Method
tc	711.24	K	Joback Method
tf	272.99	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.86	J/mol×K	518.46	Joback Method
cpg	297.54	J/mol×K	550.59	Joback Method
cpg	309.59	J/mol×K	582.72	Joback Method
cpg	321.03	J/mol×K	614.85	Joback Method
cpg	331.88	J/mol×K	646.98	Joback Method
cpg	342.18	J/mol×K	679.11	Joback Method
cpg	351.94	J/mol×K	711.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R412043&Units=SI
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

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