3-hydroxy-«beta»-ionone

Inchi: InChI=1S/C13H20O2/c1-9(14)5-6-11-10(2)12(15)7-8-13(11,3)4/h5-6,12,15H,7-8H2,1-4H
InchiKey: LICNQDPDQQOXCU-AATRIKPKSA-N
Formula: C13H20O2
SMILES: CC(=O)C=CC1=C(C)C(O)CCC1(C)C
Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
gf	-104.99	kJ/mol	Joback Method
hf	-375.18	kJ/mol	Joback Method
hfus	22.37	kJ/mol	Joback Method
hvap	68.50	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.629		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
rinpol	1676.00		NIST Webbook
rinpol	1719.00		NIST Webbook
rinpol	1676.00		NIST Webbook
rinpol	1719.00		NIST Webbook
rinpol	1676.00		NIST Webbook
rinpol	1646.00		NIST Webbook
ripol	2656.00		NIST Webbook
ripol	2675.00		NIST Webbook
ripol	2693.00		NIST Webbook
ripol	2672.00		NIST Webbook
ripol	2700.00		NIST Webbook
ripol	2700.00		NIST Webbook
ripol	2700.00		NIST Webbook
ripol	2702.00		NIST Webbook
ripol	2693.00		NIST Webbook
ripol	2641.00		NIST Webbook
ripol	2675.00		NIST Webbook
ripol	2700.00		NIST Webbook
tb	671.29	K	Joback Method
tc	875.23	K	Joback Method
tf	394.78	K	Joback Method

vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.33	J/mol×K	671.29	Joback Method
cpg	515.41	J/mol×K	705.28	Joback Method
cpg	529.82	J/mol×K	739.27	Joback Method
cpg	543.66	J/mol×K	773.26	Joback Method
cpg	557.02	J/mol×K	807.25	Joback Method
cpg	570.02	J/mol×K	841.24	Joback Method
cpg	582.75	J/mol×K	875.23	Joback Method

Sources

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=R272885&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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