3-Buten-2-one, 4-(4-hydroxy-2,2,6-trimethyl-7-oxabicyclo[4.1.0]he

Other names: 3-Hydroxy-5,6-epoxy-«beta»-ionone
4-(4-Hydroxy-2.2.6-trimethyl-7-oxabicyclo[4.1.0]-hept-1-yl)-3-buten-2-one
4-(1,2-Epoxy-4-hydroxy-2,6,6-trimethylcyclohexyl)-trans-3-buten-2-one
Inchi: InChI=1S/C13H20O3/c1-9(14)5-6-13-11(2,3)7-10(15)8-12(13,4)16-13/h5-6,10,15H,7-8H2
InchiKey: VYKLRWGPNUVKNC-AATRIKPKSA-N
Formula: C13H20O3
SMILES: CC(=O)C=CC12OC1(C)CC(O)CC2(C)C
Mol. weight [g/mol]: 224.30
CAS: 38274-01-0

Physical Properties

Property code	Value	Unit	Source
gf	-135.55	kJ/mol	Joback Method
hf	-446.76	kJ/mol	Joback Method
hfus	20.71	kJ/mol	Joback Method
hvap	68.35	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	1.840		Crippen Method
mcvol	181.320	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
rinpol	1690.20		NIST Webbook
rinpol	1715.00		NIST Webbook
rinpol	1683.00		NIST Webbook
rinpol	1737.00		NIST Webbook
ripol	2741.00		NIST Webbook
ripol	2747.00		NIST Webbook
ripol	2747.00		NIST Webbook
ripol	2739.00		NIST Webbook
ripol	2739.00		NIST Webbook
ripol	2739.00		NIST Webbook
tb	683.13	K	Joback Method
tc	896.22	K	Joback Method
tf	464.09	K	Joback Method
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.14	J/mol×K	683.13	Joback Method
cpg	546.08	J/mol×K	718.64	Joback Method
cpg	560.81	J/mol×K	754.16	Joback Method
cpg	575.66	J/mol×K	789.67	Joback Method
cpg	590.94	J/mol×K	825.19	Joback Method
cpg	606.97	J/mol×K	860.70	Joback Method
cpg	624.07	J/mol×K	896.22	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=C38274010&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

Latest version available from:
https://www.chemeo.com/cid/69-488-5/3-Buten-2-one-4-4-hydroxy-2-2-6-trimethyl-7-oxabicyclo-4-1-0-hept-1-yl.pdf
Generated by Cheméo on 2024-04-26 09:09:15.606642621 +0000 UTC m=+16411804.527219932.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.