3-oxo-retro-«alpha»-ionol

Other names: 3-oxoretro-«alpha»-ionol, isomer 2
9-hydroxymegastigma-4,6-dien-3-one
Inchi: InChI=1S/C13H20O2/c1-9-7-11(15)8-13(3,4)12(9)6-5-10(2)14/h6-7,10,14H,5,8H2,1-4H3
InchiKey: JHWWVZZGBLPJPW-UHFFFAOYSA-N
Formula: C13H20O2
SMILES: CC1=CC(=O)CC(C)(C)C1=CCC(C)O
Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
hfus	16.19	kJ/mol	Joback Method
logp	2.629		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
rinpol	1698.00		NIST Webbook
rinpol	1738.00		NIST Webbook
rinpol	1738.00		NIST Webbook
ripol	2829.00		NIST Webbook
ripol	2846.00		NIST Webbook
ripol	2850.00		NIST Webbook
ripol	2797.00		NIST Webbook
ripol	2829.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.30	J/mol×K	686.97	Joback Method
cpg	524.83	J/mol×K	721.86	Joback Method
cpg	539.71	J/mol×K	756.75	Joback Method
cpg	554.03	J/mol×K	791.64	Joback Method
cpg	567.87	J/mol×K	826.52	Joback Method
cpg	581.31	J/mol×K	861.41	Joback Method
cpg	594.44	J/mol×K	896.30	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R225220&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices