

3-oxo-retro-«alpha»-ionol (II)

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
ripol	2890.00		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

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):	
Cheméo Relay (1.0, beta):	

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R335783&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Legend

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

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