3,4-didehydro-«beta»-ionol

Other names: 3,4-dehydro-«beta»-ionol
4-(2,6,6-trimethylcyclohexa-1,3-dienyl)but-3-en-2-ol
3,4-Dydehydro «beta»-ionol
dehydro-«beta»-ionol
Inchi: InChI=1S/C13H20O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h5-8,11,14H,9H2,1-4H3/b8-7-
InchiKey: SJICFWRZYCWFOK-BQYQJAHWSA-N
Formula: C13H20O
SMILES: CC1=C(C=CC(C)O)C(C)(C)CC=C1
Mol. weight [g/mol]: 192.30

Physical Properties

Property code	Value	Unit	Source
hfus	17.40	kJ/mol	Joback Method
logp	3.226		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
rinpol	1392.00		NIST Webbook
rinpol	1397.00		NIST Webbook
rinpol	1396.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1396.00		NIST Webbook
ripol	2007.00		NIST Webbook
ripol	2013.00		NIST Webbook
ripol	2007.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.92	J/mol×K	620.81	Joback Method
cpg	472.12	J/mol×K	654.57	Joback Method
cpg	486.56	J/mol×K	688.32	Joback Method
cpg	500.33	J/mol×K	722.08	Joback Method
cpg	513.54	J/mol×K	755.84	Joback Method
cpg	526.30	J/mol×K	789.59	Joback Method
cpg	538.72	J/mol×K	823.35	Joback Method

Sources

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=R219082&Units=SI
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
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