(E)-2,3-Didehydro-«alpha»-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
ripol	2010.00		NIST Webbook
ripol	2019.00		NIST Webbook
ripol	2024.00		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

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R547718&Units=SI

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