6-Hydroxy-3-oxo-«alpha»-ionol (Vomifoliol)

Inchi: InChI=1S/C13H18O3/c1-9-7-11(15)8-12(3,4)13(9,16)6-5-10(2)14/h5-7,16H,8H2,1-4H3/b
InchiKey: JJRYPZMXNLLZFH-AATRIKPKSA-N
Formula: C13H18O3
SMILES: CC(=O)C=CC1(O)C(C)=CC(=O)CC1(C)C
Mol. weight [g/mol]: 222.28

Physical Properties

Property code	Value	Unit	Source
hfus	15.97	kJ/mol	Joback Method
logp	1.808		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
rinpol	1802.00		NIST Webbook
rinpol	1802.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.71	J/mol×K	734.37	Joback Method
cpg	540.92	J/mol×K	771.16	Joback Method
cpg	555.92	J/mol×K	807.95	Joback Method
cpg	570.90	J/mol×K	844.74	Joback Method
cpg	586.06	J/mol×K	881.53	Joback Method
cpg	601.58	J/mol×K	918.32	Joback Method
cpg	617.66	J/mol×K	955.11	Joback Method

Sources

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=R614992&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

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