4-hydroxy-«beta»-ionol

Other names: 4-Hydroxy-B-ionol
Inchi: InChI=1S/C13H22O2/c1-9-7-11(15)8-13(3,4)12(9)6-5-10(2)14/h5-6,10-11,14-15H,7-8H2,
InchiKey: JUFKQNCQDFHWFD-AATRIKPKSA-N
Formula: C13H22O2
SMILES: CC1=C(C=CC(C)O)C(C)(C)CC(O)C1
Mol. weight [g/mol]: 210.31

Physical Properties

Property code	Value	Unit	Source
hfus	21.33	kJ/mol	Joback Method
logp	2.421		Crippen Method
mcvol	186.310	ml/mol	McGowan Method
rinpol	1600.00		NIST Webbook
rinpol	1594.00		NIST Webbook
rinpol	1628.00		NIST Webbook
rinpol	1594.00		NIST Webbook
rinpol	1600.00		NIST Webbook
ripol	2593.00		NIST Webbook
ripol	2593.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.73	J/mol×K	709.16	Joback Method
cpg	555.85	J/mol×K	741.02	Joback Method
cpg	569.46	J/mol×K	772.88	Joback Method
cpg	582.63	J/mol×K	804.74	Joback Method
cpg	595.46	J/mol×K	836.61	Joback Method
cpg	608.02	J/mol×K	868.47	Joback Method
cpg	620.41	J/mol×K	900.33	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=R58842&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
ripol:	Polar retention indices