trans-«BETA»-ionone-5,6-epoxide

Inchi: InChI=1S/C13H20O2/c1-10(14)6-9-13-11(2,3)7-5-8-12(13,4)15-13/h6,9H,5,7-8H2,1-4H3/
InchiKey: ZTJZJYUGOJYHCU-RMKNXTFCSA-N
Formula: C13H20O2
SMILES: CC(=O)C=CC12OC1(C)CCCC2(C)C
Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
hfus	15.55	kJ/mol	Joback Method
logp	2.869		Crippen Method
mcvol	175.450	ml/mol	McGowan Method
ripol	1989.00		NIST Webbook
ripol	1989.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.73	J/mol×K	595.62	Joback Method
cpg	488.22	J/mol×K	634.08	Joback Method
cpg	504.61	J/mol×K	672.54	Joback Method
cpg	520.30	J/mol×K	710.99	Joback Method
cpg	535.71	J/mol×K	749.45	Joback Method
cpg	551.26	J/mol×K	787.91	Joback Method
cpg	567.34	J/mol×K	826.37	Joback Method

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R344851&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

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