.alpha.-ionone epoxide

Other names: «alpha»-Ionone epoxide (Isomer 1)
«alpha»-Ionone epoxide (Isomer 2)
Inchi: InChI=1S/C13H20O2/c1-9(14)5-6-10-12(2,3)8-7-11-13(10,4)15-11/h5-6,10-11H,7-8H2,1-
InchiKey: ODMUHAHUBCUABS-AATRIKPKSA-N
Formula: C13H20O2
SMILES: CC(=O)/C=C/C1C(C)(C)CCC2OC21C
Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
hfus	22.92	kJ/mol	Joback Method
logp	2.725		Crippen Method
mcvol	175.450	ml/mol	McGowan Method
ripol	2133.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.18	J/mol×K	590.71	Joback Method
cpg	492.47	J/mol×K	627.68	Joback Method
cpg	509.60	J/mol×K	664.66	Joback Method
cpg	525.85	J/mol×K	701.63	Joback Method
cpg	541.47	J/mol×K	738.60	Joback Method
cpg	556.73	J/mol×K	775.57	Joback Method
cpg	571.91	J/mol×K	812.55	Joback Method

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R344039&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

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