«beta»-Ionone isomer # 2

Inchi: InChI=1S/C13H20O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h7-8H,5-6,9H2,1-4H3/b8-7+
InchiKey: PSQYTAPXSHCGMF-BQYQJAHWSA-N
Formula: C13H20O
SMILES: CC(=O)C=CC1=C(C)CCCC1(C)C
Mol. weight [g/mol]: 192.30

Physical Properties

Property code	Value	Unit	Source
hfus	17.21	kJ/mol	Joback Method
ie	8.45	eV	Cheméo Relay (1.0)
logp	3.658		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
rinpol	1521.00		NIST Webbook
rinpol	1521.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.25	J/mol×K	583.78	Joback Method
cpg	455.12	J/mol×K	620.30	Joback Method
cpg	471.95	J/mol×K	656.81	Joback Method
cpg	487.87	J/mol×K	693.33	Joback Method
cpg	503.02	J/mol×K	729.85	Joback Method
cpg	517.51	J/mol×K	766.36	Joback Method
cpg	531.49	J/mol×K	802.88	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R130419&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):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices