«beta»-iso-Methyl ionone

Inchi: InChI=1S/C14H22O/c1-10-7-6-8-14(4,5)13(10)9-11(2)12(3)15/h9H,6-8H2,1-5H3/b11-9+
InchiKey: NSSHGPBKKVJJMM-PKNBQFBNSA-N
Formula: C14H22O
SMILES: CC(=O)C(C)=CC1=C(C)CCCC1(C)C
Mol. weight [g/mol]: 206.32

Physical Properties

Property code	Value	Unit	Source
hfus	18.49	kJ/mol	Joback Method
ie	8.36	eV	Cheméo Relay (1.0)
logp	4.048		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
rinpol	1904.00		NIST Webbook
rinpol	1904.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.69	J/mol×K	606.54	Joback Method
cpg	506.36	J/mol×K	643.05	Joback Method
cpg	523.99	J/mol×K	679.56	Joback Method
cpg	540.71	J/mol×K	716.07	Joback Method
cpg	556.67	J/mol×K	752.58	Joback Method
cpg	571.99	J/mol×K	789.09	Joback Method
cpg	586.80	J/mol×K	825.60	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U285402&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