3-Penten-2-one, 4-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, (E)-

Other names: (E)-4-(2',6',6'-Trimethyl-1',2'-epoxy-cyclohexyl)-3-penten-2-one (isomer 2)
Inchi: InChI=1S/C14H22O2/c1-10(9-11(2)15)14-12(3,4)7-6-8-13(14,5)16-14/h9H,6-8H2,1-5H3/
InchiKey: RNLTZJIZBIPGAV-KTKRTIGZSA-N
Formula: C14H22O2
SMILES: CC(=O)C=C(C)C12OC1(C)CCCC2(C)C
Mol. weight [g/mol]: 222.32
CAS: 89128-12-1

Physical Properties

Property code	Value	Unit	Source
gf	8.85	kJ/mol	Joback Method
hf	-304.62	kJ/mol	Joback Method
hfus	16.83	kJ/mol	Joback Method
hvap	54.29	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.259		Crippen Method
mcvol	189.540	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
rinpol	1486.00		NIST Webbook
rinpol	1486.00		NIST Webbook
tb	618.38	K	Joback Method
tc	848.73	K	Joback Method
tf	404.82	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.89	J/mol×K	618.38	Joback Method
cpg	539.16	J/mol×K	656.77	Joback Method
cpg	556.49	J/mol×K	695.16	Joback Method
cpg	573.28	J/mol×K	733.55	Joback Method
cpg	589.95	J/mol×K	771.94	Joback Method
cpg	606.92	J/mol×K	810.34	Joback Method

cpg	624.60	J/mol×K	848.73	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C89128121&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume