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

Other names: «beta»-Ionon-5,6-epoxide
«beta»-Ionone epoxide
7-Oxabicyclo[4.1.0]heptane, 3-buten-2-one deriv.
5,6-Epoxy-«beta»-ionone
4-(2,2,6-Trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-3-buten-2-one
«beta»-Ionone-5,6-epoxide
Epoxy-«beta»-ionone
«beta»-Ionone-5,6-epoxyde
5,6-«beta»-Ionone epoxide
«beta»-ionone-5,6-epoxide (trans type)
Trans-«beta»-ionone-5,6-epoxyde
(E)-«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

CAS: 23267-57-4

Physical Properties

Property code	Value	Unit	Source
gf	8.98	kJ/mol	Joback Method
hf	-274.19	kJ/mol	Joback Method
hfus	15.55	kJ/mol	Joback Method
hvap	51.98	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.869		Crippen Method
mcvol	175.450	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	1428.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1492.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1458.00		NIST Webbook
rinpol	1463.00		NIST Webbook

rinpol	1428.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1467.00		NIST Webbook
rinpol	1488.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1458.00		NIST Webbook
rinpol	1484.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1428.00		NIST Webbook
rinpol	1488.00		NIST Webbook
ripol	2002.00		NIST Webbook
ripol	1977.00		NIST Webbook
ripol	1957.00		NIST Webbook
ripol	1954.00		NIST Webbook
ripol	1940.00		NIST Webbook
ripol	1936.00		NIST Webbook
ripol	1954.00		NIST Webbook
ripol	1967.00		NIST Webbook
ripol	2002.00		NIST Webbook
ripol	1989.00		NIST Webbook
ripol	1940.00		NIST Webbook
ripol	1934.00		NIST Webbook
ripol	1968.00		NIST Webbook
tb	595.62	K	Joback Method
tc	826.37	K	Joback Method
tf	407.51	K	Joback Method
vc	0.669	m3/kmol	Joback Method

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

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=C23267574&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/63-129-9/3-Buten-2-one-4-2-2-6-trimethyl-7-oxabicyclo-4-1-0-hept-1-yl.pdf
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