Bicyclo[3.1.0]hex-3-en-2-one, 4-methyl-1-(1-methylethyl)-

Other names: 3-Thujen-2-one
Umbellulon
Umbellulone
THUJEN-2-ONE
1-Isopropyl-4-methylbicyclo[3.1.0]hex-3-en-2-one
3-Thujene-2-one
Thuj-3-en-2-one
NSC 22046
Umbellunone

Inchi: InChI=1S/C10H14O/c1-6(2)10-5-8(10)7(3)4-9(10)11/h4,6,8H,5H2,1-3H3

InchiKey: LTTVJAQLCIHAFV-UHFFFAOYSA-N

Formula: C10H14O

SMILES: CC1=CC(=O)C2(C(C)C)CC12

Mol. weight [g/mol]: 150.22

CAS: 24545-81-1

Physical Properties

Property code	Value	Unit	Source
gf	44.63	kJ/mol	Joback Method
hf	-185.56	kJ/mol	Joback Method
hfus	8.45	kJ/mol	Joback Method
hvap	41.34	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.178		Crippen Method
mcvol	127.310	ml/mol	McGowan Method
pc	3055.79	kPa	Joback Method
rinpol	1174.30		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1184.00		NIST Webbook

rinpol	1181.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1174.30		NIST Webbook
rinpol	1187.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1177.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1146.00		NIST Webbook
ripol	1610.00		NIST Webbook
ripol	1658.00		NIST Webbook
ripol	1658.00		NIST Webbook
ripol	1676.00		NIST Webbook
ripol	1616.00		NIST Webbook
ripol	1667.00		NIST Webbook
ripol	1646.00		NIST Webbook
ripol	1637.00		NIST Webbook
ripol	1666.00		NIST Webbook
ripol	1657.00		NIST Webbook
ripol	1656.00		NIST Webbook
ripol	1614.00		NIST Webbook
ripol	1657.00		NIST Webbook
tb	513.44	K	Joback Method
tc	736.91	K	Joback Method
tf	328.74	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.56	J/mol×K	513.44	Joback Method
cpg	322.25	J/mol×K	550.69	Joback Method
cpg	336.84	J/mol×K	587.93	Joback Method
cpg	350.48	J/mol×K	625.18	Joback Method
cpg	363.32	J/mol×K	662.42	Joback Method
cpg	375.49	J/mol×K	699.67	Joback Method
cpg	387.15	J/mol×K	736.91	Joback Method

Sources

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=C24545811&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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