2-Cyclopenten-1-one, 3-methyl-2-(2-pentenyl)-, (Z)-

Other names: cis-Jasmone
Jasmone
(Z)-Jasmone
3-Methyl-2-(cis-2-penten-1-yl)-2-cyclopenten-1-one
3-methyl-2-(cis-2-pentenyl)-2-cyclopenten-1-one
3-methyl-2-pent-2-enylcyclopent-2-enone

Inchi: InChI=1S/C11H16O/c1-3-4-5-6-10-9(2)7-8-11(10)12/h4-5H,3,6-8H2,1-2H3/b5-4-

InchiKey: XMLSXPIVAXONDL-PLNGDYQASA-N

Formula: C11H16O

SMILES: CCC=CCC1=C(C)CCC1=O

Mol. weight [g/mol]: 164.24

CAS: 488-10-8

Physical Properties

Property code	Value	Unit	Source
gf	54.33	kJ/mol	Joback Method
hf	-175.19	kJ/mol	Joback Method
hfus	17.27	kJ/mol	Joback Method
hvap	46.47	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	3.022		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
rinpol	1394.00		NIST Webbook
rinpol	1369.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1388.00		NIST Webbook
rinpol	1394.00		NIST Webbook
rinpol	1392.00		NIST Webbook
rinpol	1393.00		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1365.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1404.00		NIST Webbook
rinpol	1394.00		NIST Webbook
rinpol	1388.00		NIST Webbook

rinpol	1393.00	NIST Webbook
rinpol	1400.00	NIST Webbook
rinpol	1400.00	NIST Webbook
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rinpol	1405.00	NIST Webbook
rinpol	1405.00	NIST Webbook
rinpol	1393.00	NIST Webbook
rinpol	1362.00	NIST Webbook
rinpol	1394.00	NIST Webbook
rinpol	1394.00	NIST Webbook
rinpol	1402.90	NIST Webbook
rinpol	1363.90	NIST Webbook
rinpol	1376.30	NIST Webbook
rinpol	1369.00	NIST Webbook
rinpol	1398.00	NIST Webbook
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ripol	1943.00	NIST Webbook
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ripol	1914.00		NIST Webbook
ripol	1961.00		NIST Webbook
ripol	1959.00		NIST Webbook
ripol	1955.00		NIST Webbook
ripol	1953.00		NIST Webbook
ripol	1969.00		NIST Webbook
ripol	1960.00		NIST Webbook
ripol	1915.00		NIST Webbook
ripol	1984.00		NIST Webbook
ripol	1940.00		NIST Webbook
ripol	1943.00		NIST Webbook
ripol	1923.00		NIST Webbook
ripol	1947.00		NIST Webbook
ripol	1933.00		NIST Webbook
ripol	1947.00		NIST Webbook
ripol	1960.00		NIST Webbook
ripol	1961.00		NIST Webbook
ripol	1955.00		NIST Webbook
ripol	1961.00		NIST Webbook
ripol	1938.00		NIST Webbook
ripol	1973.00		NIST Webbook
ripol	1914.00		NIST Webbook
tb	552.13	K	Joback Method
tc	768.56	K	Joback Method
tf	317.81	K	Joback Method
vc	0.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.55	J/mol×K	552.13	Joback Method
cpg	364.59	J/mol×K	588.20	Joback Method
cpg	379.80	J/mol×K	624.27	Joback Method
cpg	394.21	J/mol×K	660.34	Joback Method

cpg	407.84	J/mol×K	696.41	Joback Method
cpg	420.71	J/mol×K	732.49	Joback Method
cpg	432.85	J/mol×K	768.56	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	407.70	K	1.60	NIST Webbook

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=C488108&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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume