

2H-Pyran-2-one, tetrahydro-6-(2-pentenyl)-, (Z)-

Other names:	5-Hydroxy-7(Z)-decenoic acid-«delta»-lactone Jasmine lactone Jasminlactone (Z)-7-Decen-5-olide «delta»-Jasmine lactone cis-7-Decen-5-olide Dec-7-en-5-olide, (Z)- Dec-7(Z)-en-5-olide (Z)-Dec-7-en-5-olide cis-Jasmin lactone Jasmolactone, «delta»- (Z)-dec-7-en-5-olide [jasmine lactone] (Z)-tetrahydro-6-(2-pentenyl)-2H-pyran-2-one
Inchi:	InChI=1S/C10H16O2/c1-2-3-4-6-9-7-5-8-10(11)12-9/h3-4,9H,2,5-8H2,1H3/b4-3-
InchiKey:	XPPALVZZCMPTIV-ARJAWSKDSA-N
Formula:	C10H16O2
SMILES:	CCC=CCC1CCCC(=O)O1
Mol. weight [g/mol]:	168.23
CAS:	25524-95-2

Physical Properties

Property code	Value	Unit	Source
gf	-70.72	kJ/mol	Joback Method
hf	-347.89	kJ/mol	Joback Method
hfus	21.18	kJ/mol	Joback Method
hvap	47.00	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.438		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2784.72	kPa	Joback Method
rinpol	1517.80		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1517.80		NIST Webbook
ripol	2256.00		NIST Webbook
ripol	2259.00		NIST Webbook
ripol	2245.00		NIST Webbook

ripol	2255.00		NIST Webbook
ripol	2273.00		NIST Webbook
ripol	2272.00		NIST Webbook
ripol	2274.00		NIST Webbook
ripol	2278.00		NIST Webbook
ripol	2290.00		NIST Webbook
ripol	2226.00		NIST Webbook
ripol	2253.00		NIST Webbook
ripol	2257.00		NIST Webbook
ripol	2236.00		NIST Webbook
ripol	2239.00		NIST Webbook
tb	546.68	K	Joback Method
tc	768.27	K	Joback Method
tf	299.55	K	Joback Method
vc	0.536	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.63	J/mol×K	546.68	Joback Method
cpg	370.48	J/mol×K	583.61	Joback Method
cpg	387.36	J/mol×K	620.54	Joback Method
cpg	403.30	J/mol×K	657.48	Joback Method
cpg	418.31	J/mol×K	694.41	Joback Method
cpg	432.39	J/mol×K	731.34	Joback Method
cpg	445.57	J/mol×K	768.27	Joback Method

Sources

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=C25524952&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

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
hvac:	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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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