

6-Dodecenyyl-«gamma»-lactone

Other names:	6-dodeceno-«gamma»-lactone Dihydro-5-(2-octenyl)-2(3H)-furanone 2(3H)-Furanone, dihydro-5-(2-octenyl) 6-dodecen-4-olide
Inchi:	InChI=1S/C12H20O2/c1-2-3-4-5-6-7-8-11-9-10-12(13)14-11/h6-7,11H,2-5,8-10H2,1H3/b
InchiKey:	QFXOXDSHNXAFEY-VOTSOKGWSA-N
Formula:	C12H20O2
SMILES:	CCCCC=CCC1CCC(=O)O1
Mol. weight [g/mol]:	196.29
CAS:	15456-69-6

Physical Properties

Property code	Value	Unit	Source
gf	-41.78	kJ/mol	Joback Method
hf	-383.01	kJ/mol	Joback Method
hfus	28.46	kJ/mol	Joback Method
hvap	51.28	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.219		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
rinpol	1701.00		NIST Webbook
rinpol	1661.00		NIST Webbook
rinpol	1701.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1701.00		NIST Webbook
ripol	2390.00		NIST Webbook
ripol	2390.00		NIST Webbook
ripol	2437.00		NIST Webbook
ripol	2365.00		NIST Webbook
ripol	2437.00		NIST Webbook
ripol	2365.00		NIST Webbook
ripol	2389.00		NIST Webbook
ripol	2389.00		NIST Webbook
tb	588.17	K	Joback Method
tc	795.16	K	Joback Method
tf	325.61	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.55	J/mol×K	588.17	Joback Method
cpg	468.68	J/mol×K	622.67	Joback Method
cpg	485.86	J/mol×K	657.17	Joback Method
cpg	502.11	J/mol×K	691.66	Joback Method
cpg	517.44	J/mol×K	726.16	Joback Method
cpg	531.90	J/mol×K	760.66	Joback Method
cpg	545.49	J/mol×K	795.16	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=C15456696&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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
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
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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