2(3H)-Furanone, 5-dodecyldihydro-

Other names:	Hexadecanoic acid, 4-hydroxy-, «gamma»-lactone «gamma»-Palmitolactone «gamma»-Hexadecalactone Palmito-«gamma»-lactone
Inchi:	InChI=1S/C16H30O2/c1-2-3-4-5-6-7-8-9-10-11-12-15-13-14-16(17)18-15/h15H,2-14H2,1
InchiKey:	SRIFJCOBFTWCTM-UHFFFAOYSA-N
Formula:	C16H30O2
SMILES:	CCCCCCCCCCCCC1CCC(=O)O1
Mol. weight [g/mol]:	254.41
CAS:	730-46-1

Physical Properties

Property code	Value	Unit	Source
gf	-88.32	kJ/mol	Joback Method
hf	-582.79	kJ/mol	Joback Method
hfus	38.62	kJ/mol	Joback Method
hvap	60.22	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	5.003		Crippen Method
mcvol	232.880	ml/mol	McGowan Method
pc	1540.29	kPa	Joback Method
rinpol	2104.30		NIST Webbook
rinpol	2106.00		NIST Webbook
rinpol	2120.00		NIST Webbook
rinpol	2104.30		NIST Webbook
rinpol	2106.00		NIST Webbook
ripol	2857.00		NIST Webbook
ripol	2857.00		NIST Webbook
ripol	2810.00		NIST Webbook
ripol	2810.00		NIST Webbook
ripol	2857.00		NIST Webbook
tb	675.53	K	Joback Method
tc	865.32	K	Joback Method
tf	375.77	K	Joback Method
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	687.36	J/mol×K	675.53	Joback Method
cpg	707.39	J/mol×K	707.16	Joback Method
cpg	726.40	J/mol×K	738.79	Joback Method
cpg	744.40	J/mol×K	770.43	Joback Method
cpg	761.43	J/mol×K	802.06	Joback Method
cpg	777.48	J/mol×K	833.69	Joback Method
cpg	792.59	J/mol×K	865.32	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=C730461&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

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