3(2H)-FURANONE, 5-METHYL-2-OCTYL-

Other names: 2,3-Dihydro-2-n-octyl-5-methyl-furan-3-one
2,3-Dihydro-5-methyl-2-n-octylfuran-3-one
2H-Furan-3-one, 5-methyl-2-octyl
Inchi: InChI=1S/C13H22O2/c1-3-4-5-6-7-8-9-13-12(14)10-11(2)15-13/h10,13H,3-9H2,1-2H3
InchiKey: ZLLDSWALGJWTSW-UHFFFAOYSA-N
Formula: C13H22O2
SMILES: CCCCCCCCC1OC(C)=CC1=O
Mol. weight [g/mol]: 210.32

Physical Properties

Property code	Value	Unit	Source
hf	-454.56	kJ/mol	Cheméo Relay (1.0)
hfus	31.68	kJ/mol	Joback Method
hvap	73.32	kJ/mol	Cheméo Relay (1.0)
ie	8.98	eV	Cheméo Relay (1.0)
logp	3.609		Crippen Method
mcvol	186.310	ml/mol	McGowan Method
rinpol	1626.00		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1622.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1652.80		NIST Webbook
rinpol	1652.80		NIST Webbook
rinpol	1626.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.23	J/mol×K	611.03	Joback Method
cpg	519.02	J/mol×K	644.12	Joback Method
cpg	535.96	J/mol×K	677.21	Joback Method
cpg	552.04	J/mol×K	710.30	Joback Method
cpg	567.27	J/mol×K	743.39	Joback Method
cpg	581.66	J/mol×K	776.48	Joback Method

cpg	595.23	J/mol×K	809.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57877722&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

Latest version available from:
https://www.chemeo.com/cid/93-212-3/3-2H-FURANONE-5-METHYL-2-OCTYL.pdf
Generated by Cheméo on 2026-07-22 05:25:26.912181808 +0000 UTC m=+209022.754067293.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.