6-Undecyltetrahydro-2H-pyran-2-one

Other names:	Hexadecalactone
	2H-Pyran-2-one, tetrahydro-6-undecyl-
	tetrahydro-6-undecyl-2H-pyran-2-one
	6-Undecyltetrahydro-2H-pyran-2-one
Inchi:	InChI=1S/C16H30O2/c1-2-3-4-5-6-7-8-9-10-12-15-13-11-14-16(17)18-15/h15H,2-14H2,1
InchiKey:	ZMJKQSSFLIFELJ-UHFFFAOYSA-N
Formula:	C16H30O2
SMILES:	CCCCCCCCCCCC1CCCC(=O)O1
Mol. weight [g/mol]:	254.41

Physical Properties

Property code	Value	Unit	Source
af	0.7539		Cheméo Relay (1.0)
gf	-177.88	kJ/mol	Joback Method
hf	-638.05	kJ/mol	Cheméo Relay (1.0)
hfus	37.60	kJ/mol	Joback Method
hvap	97.03	kJ/mol	Cheméo Relay (1.0)
ie	9.82	eV	Cheméo Relay (1.0)
logp	5.003		Crippen Method
mcvol	232.880	ml/mol	McGowan Method
pc	1486.14	kPa	Joback Method
rinpol	2154.00		NIST Webbook
rinpol	2154.00		NIST Webbook
rinpol	2141.90		NIST Webbook
rinpol	2141.90		NIST Webbook
tb	629.56	K	Cheméo Relay (1.0)
tc	807.56	K	Cheméo Relay (1.0)
tf	288.38	K	Cheméo Relay (1.0)
vc	0.890	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.61	J/mol×K	634.91	Joback Method

cpg	675.89	J/mol×K	664.57	Joback Method
cpg	694.21	J/mol×K	694.24	Joback Method
cpg	711.60	J/mol×K	723.90	Joback Method
cpg	728.09	J/mol×K	753.57	Joback Method
cpg	743.72	J/mol×K	783.23	Joback Method
cpg	758.51	J/mol×K	812.90	Joback Method
dvisc	0.0035013	Pa×s	326.83	Joback Method
dvisc	0.0015873	Pa×s	378.18	Joback Method
dvisc	0.0008695	Pa×s	429.52	Joback Method
dvisc	0.0005416	Pa×s	480.87	Joback Method
dvisc	0.0003696	Pa×s	532.22	Joback Method
dvisc	0.0002698	Pa×s	583.56	Joback Method
dvisc	0.0002072	Pa×s	634.91	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7370447&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

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume