

«delta»-hexadecalactone

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
CAS:	7370-44-7

Physical Properties

Property code	Value	Unit	Source
gf	-100.42	kJ/mol	Joback Method
hf	-588.95	kJ/mol	Joback Method
hfus	36.52	kJ/mol	Joback Method
hvap	60.40	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	5.003		Crippen Method
mcvol	232.880	ml/mol	McGowan Method
pc	1570.96	kPa	Joback Method
rinpol	2141.90		NIST Webbook
rinpol	2154.00		NIST Webbook
rinpol	2154.00		NIST Webbook
rinpol	2141.90		NIST Webbook
tb	679.80	K	Joback Method
tc	874.67	K	Joback Method
tf	372.25	K	Joback Method
vc	0.892	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	690.53	J/mol×K	679.80	Joback Method

cpg	711.31	J/mol×K	712.28	Joback Method
cpg	730.98	J/mol×K	744.76	Joback Method
cpg	749.56	J/mol×K	777.24	Joback Method
cpg	767.05	J/mol×K	809.71	Joback Method
cpg	783.48	J/mol×K	842.19	Joback Method
cpg	798.85	J/mol×K	874.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7370447&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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

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