6-Undecyl-5,6-dihydro-2H-pyran-2-one

Inchi: InChI=1S/C16H28O2/c1-2-3-4-5-6-7-8-9-10-12-15-13-11-14-16(17)18-15/h11,14-15H,2-1
InchiKey: LIIXNZRSHIMJDW-UHFFFAOYSA-N
Formula: C16H28O2
SMILES: CCCCCCCCCCCC1CC=CC(=O)O1
Mol. weight [g/mol]: 252.39
CAS: 81017-06-3

Physical Properties

Property code	Value	Unit	Source
gf	-70.46	kJ/mol	Joback Method
hf	-531.17	kJ/mol	Joback Method
hfus	37.74	kJ/mol	Joback Method
hvap	60.69	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.779		Crippen Method
mcvol	228.580	ml/mol	McGowan Method
pc	1616.77	kPa	Joback Method
rinpol	2122.90		NIST Webbook
rinpol	2122.90		NIST Webbook
tb	678.96	K	Joback Method
tc	875.22	K	Joback Method
tf	373.01	K	Joback Method
vc	0.878	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.91	J/mol×K	678.96	Joback Method
cpg	686.82	J/mol×K	711.67	Joback Method
cpg	705.64	J/mol×K	744.38	Joback Method
cpg	723.39	J/mol×K	777.09	Joback Method
cpg	740.10	J/mol×K	809.80	Joback Method
cpg	755.77	J/mol×K	842.51	Joback Method
cpg	770.42	J/mol×K	875.22	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=C81017063&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume