

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

Inchi:	InChI=1S/C8H12O2/c1-2-4-7-5-3-6-8(9)10-7/h3,6-7H,2,4-5H2,1H3
InchiKey:	ZFFLYUGDQAHVSE-UHFFFAOYSA-N
Formula:	C8H12O2
SMILES:	CCCC1CC=CC(=O)O1
Mol. weight [g/mol]:	140.18
CAS:	16400-69-4

Physical Properties

Property code	Value	Unit	Source
gf	-137.82	kJ/mol	Joback Method
hf	-366.05	kJ/mol	Joback Method
hfus	17.02	kJ/mol	Joback Method
hvap	42.88	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.658		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3384.14	kPa	Joback Method
rinpol	1267.50		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1267.50		NIST Webbook
ripol	2005.00		NIST Webbook
ripol	2005.00		NIST Webbook
tb	495.92	K	Joback Method
tc	717.03	K	Joback Method
tf	282.85	K	Joback Method
vc	0.430	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.71	J/molxK	495.92	Joback Method
cpg	275.87	J/molxK	532.77	Joback Method
cpg	290.33	J/molxK	569.62	Joback Method

cpg	304.07	J/mol×K	606.47	Joback Method
cpg	317.10	J/mol×K	643.33	Joback Method
cpg	329.40	J/mol×K	680.18	Joback Method
cpg	340.96	J/mol×K	717.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16400694&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
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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