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

Inchi: InChI=1S/C7H10O2/c1-2-6-4-3-5-7(8)9-6/h3,5-6H,2,4H2,1H3
InchiKey: PBTYTLMBTXXZJF-UHFFFAOYSA-N
Formula: C7H10O2
SMILES: CCC1CC=CC(=O)O1
Mol. weight [g/mol]: 126.15
CAS: 19895-35-3

Physical Properties

Property code	Value	Unit	Source
gf	-146.24	kJ/mol	Joback Method
hf	-345.41	kJ/mol	Joback Method
hfus	14.43	kJ/mol	Joback Method
hvap	40.65	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.268		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
pc	3796.32	kPa	Joback Method
rinpol	1160.20		NIST Webbook
rinpol	1160.20		NIST Webbook
tb	473.04	K	Joback Method
tc	697.80	K	Joback Method
tf	271.58	K	Joback Method
vc	0.374	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.82	J/mol×K	473.04	Joback Method
cpg	231.80	J/mol×K	510.50	Joback Method
cpg	245.14	J/mol×K	547.96	Joback Method
cpg	257.86	J/mol×K	585.42	Joback Method
cpg	269.93	J/mol×K	622.88	Joback Method
cpg	281.34	J/mol×K	660.34	Joback Method
cpg	292.08	J/mol×K	697.80	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19895353&Units=SI

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