2H-Pyran-2-one, 6-ethyltetrahydro-

Other names:	Heptanoic acid, 5-hydroxy-, «delta»-lactone
	5-Hydroxyheptanoic acid lactone
	6-Ethyltetrahydro-2H-pyran-2-one
	«delta»-Heptalactone
	«delta»-Heptanolide
Inchi:	InChI=1S/C7H12O2/c1-2-6-4-3-5-7(8)9-6/h6H,2-5H2,1H3
InchiKey:	JFVQYQDTHWLYHG-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	CCC1CCCC(=O)O1
Mol. weight [g/mol]:	128.17
CAS:	3301-90-4

Physical Properties

Property code	Value	Unit	Source
gf	-176.20	kJ/mol	Joback Method
hf	-403.19	kJ/mol	Joback Method
hfus	13.21	kJ/mol	Joback Method
hvap	40.36	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	1.492		Crippen Method
mcvol	106.070	ml/mol	McGowan Method
pc	3633.35	kPa	Joback Method
rinpol	1147.00		NIST Webbook
ripol	1976.00		NIST Webbook
tb	473.88	K	Joback Method
tc	696.30	K	Joback Method
tf	270.82	K	Joback Method
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.60	J/mol×K	473.88	Joback Method
cpg	248.91	J/mol×K	510.95	Joback Method

cpg	263.56	J/mol×K	548.02	Joback Method
cpg	277.54	J/mol×K	585.09	Joback Method
cpg	290.83	J/mol×K	622.16	Joback Method
cpg	303.41	J/mol×K	659.23	Joback Method
cpg	315.29	J/mol×K	696.30	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=C3301904&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume