2H-Pyran-2-one, tetrahydro-6,6-dimethyl-

Other names: 5-Methyl-5-hydroxyhexanoic acid lactone
5-Methylhexan-5-olide
Tetrahydro-6,6-dimethyl-2H-pyran-2-one
Inchi: InChI=1S/C7H12O2/c1-7(2)5-3-4-6(8)9-7/h3-5H2,1-2H3
InchiKey: NALPFDQXLZMHJD-UHFFFAOYSA-N
Formula: C7H12O2
SMILES: CC1(C)CCCC(=O)O1
Mol. weight [g/mol]: 128.17
CAS: 2610-95-9

Physical Properties

Property code	Value	Unit	Source
gf	-181.69	kJ/mol	Joback Method
hf	-387.95	kJ/mol	Joback Method
hfus	6.91	kJ/mol	Joback Method
hvap	39.21	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	1.492		Crippen Method
mcvol	106.070	ml/mol	McGowan Method
pc	3838.78	kPa	Joback Method
rinpol	848.00		NIST Webbook
tb	474.12	K	Joback Method
tc	706.63	K	Joback Method
tf	294.72	K	Joback Method
vc	0.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.15	J/mol×K	474.12	Joback Method
cpg	249.52	J/mol×K	512.87	Joback Method
cpg	263.95	J/mol×K	551.62	Joback Method
cpg	277.51	J/mol×K	590.38	Joback Method
cpg	290.31	J/mol×K	629.13	Joback Method

cpg	302.43	J/mol×K	667.88	Joback Method
cpg	313.96	J/mol×K	706.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2610959&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume