

Tetrahydro-5,6-dimethyl-2H-pyran-2-one

Inchi:	InChI=1S/C7H12O2/c1-5-3-4-7(8)9-6(5)2/h5-6H,3-4H2,1-2H3
InchiKey:	HAXARIVGMMVELD-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	CC1CCC(=O)OC1C
Mol. weight [g/mol]:	128.17

Physical Properties

Property code	Value	Unit	Source
gf	-183.91	kJ/mol	Joback Method
hf	-423.53	kJ/mol	Joback Method
hfus	14.28	kJ/mol	Joback Method
hvap	40.05	kJ/mol	Joback Method
log10ws	-1.38		Crippen Method
logp	1.348		Crippen Method
mcvol	106.070	ml/mol	McGowan Method
pc	3493.01	kPa	Joback Method
ripol	1855.00		NIST Webbook
ripol	1855.00		NIST Webbook
tb	469.21	K	Joback Method
tc	691.39	K	Joback Method
tf	266.58	K	Joback Method
vc	0.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.42	J/molxK	469.21	Joback Method
cpg	250.08	J/molxK	506.24	Joback Method
cpg	265.11	J/molxK	543.27	Joback Method
cpg	279.49	J/molxK	580.30	Joback Method
cpg	293.21	J/molxK	617.33	Joback Method
cpg	306.23	J/molxK	654.36	Joback Method
cpg	318.55	J/molxK	691.39	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R576395&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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