

6-Methyloxan-2-one

Inchi:	InChI=1S/C6H10O2/c1-5-3-2-4-6(7)8-5/h5H,2-4H2,1H3
InchiKey:	RZTOWFMDBDPERY-UHFFFAOYSA-N
Formula:	C6H10O2
SMILES:	CC1CCCC(=O)O1
Mol. weight [g/mol]:	114.14

Physical Properties

Property code	Value	Unit	Source
gf	-184.62	kJ/mol	Joback Method
hf	-382.55	kJ/mol	Joback Method
hfus	10.62	kJ/mol	Joback Method
hvap	38.14	kJ/mol	Joback Method
log10ws	-1.20		Crippen Method
logp	1.102		Crippen Method
mcvol	91.980	ml/mol	McGowan Method
pc	4093.38	kPa	Joback Method
rinpol	1100.00		NIST Webbook
rinpol	1100.00		NIST Webbook
tb	451.00	K	Joback Method
tc	676.91	K	Joback Method
tf	259.55	K	Joback Method
vc	0.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.86	J/molxK	451.00	Joback Method
cpg	205.87	J/molxK	488.65	Joback Method
cpg	219.30	J/molxK	526.30	Joback Method
cpg	232.15	J/molxK	563.96	Joback Method
cpg	244.40	J/molxK	601.61	Joback Method
cpg	256.02	J/molxK	639.26	Joback Method
cpg	267.01	J/molxK	676.91	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=R606654&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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