Cyclopentanone ethylene ketal

Other names: 1,4-Dioxaspiro[4.4]nonane
Inchi: InChI=1S/C7H12O2/c1-2-4-7(3-1)8-5-6-9-7/h1-6H2
InchiKey: IJDXSTIWUARVEK-UHFFFAOYSA-N
Formula: C7H12O2
SMILES: C1CCC2(C1)OCCO2
Mol. weight [g/mol]: 128.17
CAS: 176-32-9

Physical Properties

Property code	Value	Unit	Source
gf	-76.76	kJ/mol	Joback Method
hf	-289.11	kJ/mol	Joback Method
hfus	12.44	kJ/mol	Joback Method
hvap	47.60 ± 0.50	kJ/mol	NIST Webbook
log10ws	-1.32		Crippen Method
logp	1.304		Crippen Method
mcvol	99.510	ml/mol	McGowan Method
pc	4474.22	kPa	Joback Method
tb	444.66	K	Joback Method
tc	675.93	K	Joback Method
tf	275.25	K	Joback Method
vc	0.358	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.24	J/mol×K	444.66	Joback Method
cpg	236.21	J/mol×K	483.21	Joback Method
cpg	251.66	J/mol×K	521.75	Joback Method
cpg	265.77	J/mol×K	560.30	Joback Method
cpg	278.71	J/mol×K	598.84	Joback Method
cpg	290.64	J/mol×K	637.39	Joback Method
cpg	301.74	J/mol×K	675.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C176329&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume