1,4-Dioxaspiro[4.4]non-6-ene

Other names:	2-Cyclopenten-1-one ethylene ketal
	cyclopent-2-en-1-one-ethyleneacetal
Inchi:	InChI=1S/C7H10O2/c1-2-4-7(3-1)8-5-6-9-7/h1,3H,2,4-6H2
InchiKey:	ATFWVBMLTLPOHI-UHFFFAOYSA-N
Formula:	C7H10O2
SMILES:	C1=CC2(CC1)OCCO2
Mol. weight [g/mol]:	126.15
CAS:	695-56-7

Physical Properties

Property code	Value	Unit	Source
gf	-46.80	kJ/mol	Joback Method
hf	-231.33	kJ/mol	Joback Method
hfus	13.67	kJ/mol	Joback Method
hvap	39.99	kJ/mol	Joback Method
log10ws	-1.18		Crippen Method
logp	1.079		Crippen Method
mcvol	95.210	ml/mol	McGowan Method
pc	4697.74	kPa	Joback Method
tb	443.82	K	Joback Method
tc	677.63	K	Joback Method
tf	276.01	K	Joback Method
vc	0.344	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.65	J/mol×K	443.82	Joback Method
cpg	220.21	J/mol×K	482.79	Joback Method
cpg	234.28	J/mol×K	521.76	Joback Method
cpg	247.04	J/mol×K	560.72	Joback Method
cpg	258.66	J/mol×K	599.69	Joback Method
cpg	269.32	J/mol×K	638.66	Joback Method
cpg	279.19	J/mol×K	677.63	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	333.70	K	2.10	NIST Webbook

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=C695567&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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