2,4,8,10-Tetraoxaspiro[5.5]undecane

Other names:	Formaldehyde, cyclic diacetal with pentaerythritol
	Pentaerythritol bisformal
	Pentaerythritol cyclic diformal
	Pentaerythritol diformal
	Pentaerythritol, bis(cyclic acetal) with formaldehyde-
	Pentaerythritol, dimethylene-
	5,5'-Spirobi-m-dioxane
	5,5'-Spirobi-1,3-dioxane
	NSC 139455
Inchi:	InChI=1S/C7H12O4/c1-7(2-9-5-8-1)3-10-6-11-4-7/h1-6H2
InchiKey:	BGCSUUSPRCDKBQ-UHFFFAOYSA-N
Formula:	C7H12O4
SMILES:	C1OCC2(CO1)COCOC2
Mol. weight [g/mol]:	160.17
CAS:	126-54-5

Physical Properties

Property code	Value	Unit	Source
chs	-3767.00	kJ/mol	NIST Webbook
gf	-273.20	kJ/mol	Joback Method
hf	-565.43	kJ/mol	Joback Method
hfus	24.20	kJ/mol	Joback Method
hsub	73.00 ± 2.00	kJ/mol	NIST Webbook
hvap	49.06	kJ/mol	Joback Method
log10ws	0.36		Crippen Method
logp	-0.019		Crippen Method
mcvol	111.250	ml/mol	McGowan Method
pc	4672.09	kPa	Joback Method
tb	507.10	K	Joback Method
tc	753.39	K	Joback Method
tf	321.35	K	Joback Method
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.52	J/mol×K	507.10	Joback Method
cpg	295.57	J/mol×K	548.15	Joback Method
cpg	311.20	J/mol×K	589.20	Joback Method
cpg	325.60	J/mol×K	630.25	Joback Method
cpg	338.92	J/mol×K	671.29	Joback Method
cpg	351.34	J/mol×K	712.34	Joback Method
cpg	363.04	J/mol×K	753.39	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	354.70	K	0.10	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=C126545&Units=SI

Legend

chs: Standard solid enthalpy of combustion
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
hsub: Enthalpy of sublimation 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