1,5-Dioxaspiro[5.5]undecane, 3,3-dimethyl-

Other names:	Cyclohexanone, 2,2-dimethyl-1,3-propanediol ketal
	3,3-dimethyl-1,5-dioxaspiro[5.5]undecane
Inchi:	InChI=1S/C11H20O2/c1-10(2)8-12-11(13-9-10)6-4-3-5-7-11/h3-9H2,1-2H3
InchiKey:	QIFSGRPJUXQGMD-UHFFFAOYSA-N
Formula:	C11H20O2
SMILES:	CC1(C)COC2(CCCCC2)OC1
Mol. weight [g/mol]:	184.28
CAS:	707-29-9

Physical Properties

Property code	Value	Unit	Source
gf	-80.48	kJ/mol	Joback Method
hf	-389.09	kJ/mol	Joback Method
hfus	13.38	kJ/mol	Joback Method
hvap	47.48	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	2.720		Crippen Method
mcvol	155.870	ml/mol	McGowan Method
pc	3028.94	kPa	Joback Method
tb	540.29	K	Joback Method
tc	783.19	K	Joback Method
tf	332.95	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.92	J/mol×K	540.29	Joback Method
cpg	425.96	J/mol×K	580.77	Joback Method
cpg	446.31	J/mol×K	621.26	Joback Method
cpg	465.25	J/mol×K	661.74	Joback Method
cpg	483.09	J/mol×K	702.22	Joback Method
cpg	500.12	J/mol×K	742.71	Joback Method
cpg	516.64	J/mol×K	783.19	Joback Method

hvapt	59.00 ± 0.60	kJ/mol	303.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C707299&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvapt:	Enthalpy of vaporization at a given temperature
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

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