

1,4-Dioxaspiro[4.5]decane

Other names:	Cyclohexanone ethylene acetal
	Cyclohexanone ethylene ketal
	Spiro[cyclohexane-1,2'-[1,3]dioxolane]
	2,2-Pentamethylene-1,3-dioxolane
	(Ethylenedioxy)cyclohexane
Inchi:	Cyclohexanone ethylene ketal
	InChI=1S/C8H14O2/c1-2-4-8(5-3-1)9-6-7-10-8/h1-7H2
InchiKey:	GZGPRYZKQBQ-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	C1CCC2(CC1)OCCO2
Mol. weight [g/mol]:	142.20
CAS:	177-10-6

Physical Properties

Property code	Value	Unit	Source
gf	-80.44	kJ/mol	Joback Method
hf	-315.91	kJ/mol	Joback Method
hfus	12.93	kJ/mol	Joback Method
hvap	50.60 ± 0.60	kJ/mol	NIST Webbook
ie	8.80	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
log10ws	-1.74		Crippen Method
logp	1.694		Crippen Method
mcvol	113.600	ml/mol	McGowan Method
pc	4077.71	kPa	Joback Method
tb	471.81	K	Joback Method
tc	708.72	K	Joback Method
tf	283.00	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.95	J/mol×K	471.81	Joback Method

cpg	280.75	J/mol×K	511.30	Joback Method
cpg	297.98	J/mol×K	550.78	Joback Method
cpg	313.81	J/mol×K	590.27	Joback Method
cpg	328.43	J/mol×K	629.75	Joback Method
cpg	342.01	J/mol×K	669.24	Joback Method
cpg	354.71	J/mol×K	708.72	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	346.20	K	2.10	NIST Webbook

Sources

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=C177106&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie:	Ionization energy
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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