

7,8-Dioxabicyclo[4.2.2]decane

Other names:	7,8-Dioxabicyclo(4,2,2)decane
Inchi:	InChI=1S/C8H14O2/c1-2-4-8-6-5-7(3-1)9-10-8/h7-8H,1-6H2
InchiKey:	GRPFSWFCSGHVIB-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	C1CCC2CCC(C1)OO2
Mol. weight [g/mol]:	142.20
CAS:	52965-57-8

Physical Properties

Property code	Value	Unit	Source
gf	-82.66	kJ/mol	Joback Method
hf	-351.49	kJ/mol	Joback Method
hfus	20.30	kJ/mol	Joback Method
hvap	42.94	kJ/mol	Joback Method
ie	9.06	eV	NIST Webbook
ie	9.05	eV	NIST Webbook
log10ws	-2.35		Crippen Method
logp	2.040		Crippen Method
mcvol	113.600	ml/mol	McGowan Method
pc	3699.95	kPa	Joback Method
tb	466.90	K	Joback Method
tc	693.20	K	Joback Method
tf	254.86	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.74	J/molxK	466.90	Joback Method
cpg	280.75	J/molxK	504.62	Joback Method
cpg	298.58	J/molxK	542.33	Joback Method
cpg	315.26	J/molxK	580.05	Joback Method
cpg	330.84	J/molxK	617.77	Joback Method
cpg	345.38	J/molxK	655.48	Joback Method

cpg	358.92	J/mol×K	693.20	Joback Method
dvisc	0.0056174	Paxs	254.86	Joback Method
dvisc	0.0029622	Paxs	290.20	Joback Method
dvisc	0.0017949	Paxs	325.54	Joback Method
dvisc	0.0011997	Paxs	360.88	Joback Method
dvisc	0.0008616	Paxs	396.22	Joback Method
dvisc	0.0006533	Paxs	431.56	Joback Method
dvisc	0.0005165	Paxs	466.90	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C52965578&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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