

7,7-dimethyl-6,8-dioxa-bicyclo[3.2.1]octane

Inchi:

InChI=1S/C8H14O2/c1-8(2)6-4-3-5-7(9-6)10-8/h6-7H,3-5H2,1-2H3

InchiKey:

CZXPPWHTHPJSCK-UHFFFAOYSA-N

Formula:

C8H14O2

SMILES:

CC1(C)OC2CCCC1O2

Mol. weight [g/mol]:

142.20

Physical Properties

Property code	Value	Unit	Source
gf	-71.66	kJ/mol	Joback Method
hf	-344.27	kJ/mol	Joback Method
hfus	19.28	kJ/mol	Joback Method
hvap	41.13	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	1.690		Crippen Method
mcvol	113.600	ml/mol	McGowan Method
pc	3534.66	kPa	Joback Method
ripol	1302.00		NIST Webbook
ripol	1302.00		NIST Webbook
ripol	1298.00		NIST Webbook
tb	453.93	K	Joback Method
tc	672.14	K	Joback Method
tf	281.56	K	Joback Method
vc	0.420	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.69	J/mol×K	453.93	Joback Method
cpg	281.25	J/mol×K	490.30	Joback Method
cpg	297.46	J/mol×K	526.67	Joback Method
cpg	312.46	J/mol×K	563.03	Joback Method
cpg	326.38	J/mol×K	599.40	Joback Method
cpg	339.37	J/mol×K	635.77	Joback Method
cpg	351.56	J/mol×K	672.14	Joback Method

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=R210203&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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