

2«alpha»,4«alpha»-Dimethyl-6«beta»-vinyl-1,3-dioxane

Inchi:	InChI=1S/C8H14O2/c1-4-8-5-6(2)9-7(3)10-8/h4,6-8H,1,5H2,2-3H3/t6-,7-,8-/m0/s1
InchiKey:	JQHFBPIKCRAJQ-FXQIFTODSA-N
Formula:	C8H14O2
SMILES:	C=CC1CC(C)OC(C)O1
Mol. weight [g/mol]:	142.20
CAS:	42411-78-9

Physical Properties

Property code	Value	Unit	Source
gf	-58.89	kJ/mol	Joback Method
hf	-333.38	kJ/mol	Joback Method
hfus	25.13	kJ/mol	Joback Method
hvap	41.56	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.712		Crippen Method
mvol	120.160	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
tb	443.23	K	Joback Method
tc	647.63	K	Joback Method
tf	230.20	K	Joback Method
vc	0.438	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.44	J/molxK	443.23	Joback Method
cpg	276.92	J/molxK	477.30	Joback Method
cpg	292.65	J/molxK	511.36	Joback Method
cpg	307.64	J/molxK	545.43	Joback Method
cpg	321.90	J/molxK	579.50	Joback Method
cpg	335.43	J/molxK	613.57	Joback Method
cpg	348.25	J/molxK	647.63	Joback Method
dvisc	0.0032862	Paxs	230.20	Joback Method
dvisc	0.0017544	Paxs	265.70	Joback Method

dvisc	0.0010860	Paxs	301.21	Joback Method
dvisc	0.0007438	Paxs	336.72	Joback Method
dvisc	0.0005475	Paxs	372.22	Joback Method
dvisc	0.0004252	Paxs	407.73	Joback Method
dvisc	0.0003438	Paxs	443.23	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C42411789&Units=SI>

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>

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
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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