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

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: JQHFVBPIKCRAJQ-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
mcvol	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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0010860	Pa×s	301.21	Joback Method
dvisc	0.0007438	Pa×s	336.72	Joback Method
dvisc	0.0005475	Pa×s	372.22	Joback Method
dvisc	0.0004252	Pa×s	407.73	Joback Method
dvisc	0.0003438	Pa×s	443.23	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=C42411789&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
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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