

1,3-Dioxolane-4-methanol, 2,2-dimethyl-, (S)-

Other names:	(S)-(+)-2,2-Dimethyl-1,3-dioxolane-4-methanol (2,2-Dimethyl-1,3-dioxolan-4-yl)methanol, (L)- (+)-Solketal (S)-2,2-dimethyl-1,3-dioxolane-4-methanol L-Acetone glycerol
Inchi:	InChI=1S/C6H12O3/c1-6(2)8-4-5(3-7)9-6/h5,7H,3-4H2,1-2H3/t5-/m1/s1
InchiKey:	RNVYQYLELCKWAN-RXMQYKEDSA-N
Formula:	C6H12O3
SMILES:	CC1(C)OCC(CO)O1
Mol. weight [g/mol]:	132.16
CAS:	22323-82-6

Physical Properties

Property code	Value	Unit	Source
chl	-3386.00	kJ/mol	NIST Webbook
gf	-286.07	kJ/mol	Joback Method
hf	-528.02	kJ/mol	Joback Method
hfus	20.05	kJ/mol	Joback Method
hvap	53.45	kJ/mol	Joback Method
log10ws	-0.39		Crippen Method
logp	0.130		Crippen Method
mcvol	102.150	ml/mol	McGowan Method
pc	4283.05	kPa	Joback Method
tb	493.61	K	Joback Method
tc	688.06	K	Joback Method
tf	301.90	K	Joback Method
vc	0.370	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.77	J/molxK	493.61	Joback Method
cpg	259.23	J/molxK	526.02	Joback Method
cpg	269.97	J/molxK	558.43	Joback Method

cpg	280.08	J/mol×K	590.84	Joback Method
cpg	289.63	J/mol×K	623.24	Joback Method
cpg	298.69	J/mol×K	655.65	Joback Method
cpg	307.33	J/mol×K	688.06	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	355.70	K	1.90	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22323826&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

chl:	Standard liquid enthalpy of combustion
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
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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