(R)-(-)-2,2-Dimethyl-1,3-dioxolane-4-methanol

Other names:	(2,2-Dimethyl-1,3-dioxolan-4-yl)methanol, D- D-Acetone glycerol 1,3-Dioxolane-4-methanol, 2,2-dimethyl-, (R)- 1,3-Dioxolane-4-methanol, 2,2-dimethyl-, (4R)-
Inchi:	InChI=1S/C6H12O3/c1-6(2)8-4-5(3-7)9-6/h5,7H,3-4H2,1-2H3/t5-/m0/s1
InchiKey:	RNVYQYLELCKWAN-YFKPBYRVSA-N
Formula:	C6H12O3
SMILES:	CC1(C)OCC(CO)O1
Mol. weight [g/mol]:	132.16
CAS:	14347-78-5

Physical Properties

Property code	Value	Unit	Source
chl	-3390.00	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/mol×K	493.61	Joback Method
cpg	259.23	J/mol×K	526.02	Joback Method
cpg	269.97	J/mol×K	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	345.70	K	1.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14347785&Units=SI
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

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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