

1,3-Dioxolane-4-carboxaldehyde, 2,2-dimethyl-, (R)-

Other names:	2,2-Dimethyl-1,3-dioxolane-4-carbaldehyde, (D)- Acetone D-glyceraldehyde (R)-(+)-Glyceraldehyde acetonide NSC 89869
Inchi:	InChI=1S/C6H10O3/c1-6(2)8-4-5(3-7)9-6/h3,5H,4H2,1-2H3
InchiKey:	YSGPYVWACGYQDJ-UHFFFAOYSA-N
Formula:	C6H10O3
SMILES:	CC1(C)OCC(C=O)O1
Mol. weight [g/mol]:	130.14
CAS:	15186-48-8

Physical Properties

Property code	Value	Unit	Source
chl	-3030.00	kJ/mol	NIST Webbook
gf	-248.77	kJ/mol	Joback Method
hf	-461.37	kJ/mol	Joback Method
hfus	18.25	kJ/mol	Joback Method
hvap	43.49	kJ/mol	Joback Method
log10ws	-0.40		Crippen Method
logp	0.337		Crippen Method
mcvol	97.850	ml/mol	McGowan Method
pc	4183.90	kPa	Joback Method
tb	450.09	K	Joback Method
tc	662.28	K	Joback Method
tf	283.08	K	Joback Method
vc	0.368	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.95	J/mol×K	450.09	Joback Method
cpg	229.44	J/mol×K	485.45	Joback Method
cpg	241.02	J/mol×K	520.82	Joback Method
cpg	251.79	J/mol×K	556.18	Joback Method

cpg	261.84	J/mol×K	591.55	Joback Method
cpg	271.25	J/mol×K	626.91	Joback Method
cpg	280.13	J/mol×K	662.28	Joback Method

Sources

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=C15186488&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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