Methyl «alpha»,«beta»-isopropylidene-D-glycerate

Other names: Methyl (R)-(+)-2,2-dimethyl-1,3-dioxolane-4-carboxylate
1,3-Dioxolane-4-carboxylic acid, 2,2-dimethyl-, methyl ester, (R)-
1,3-Dioxolane-4-carboxylic acid, 2,2-dimethyl-, methyl ester, (4R)-
(R)-2,2-Dimethyl-(1,3)-dioxolane-4-carboxylic methyl ester

Inchi: InChI=1S/C7H12O4/c1-7(2)10-4-5(11-7)6(8)9-3/h5H,4H2,1-3H3

InchiKey: DOWWCCDWPKGNGX-UHFFFAOYSA-N

Formula: C7H12O4

SMILES: COC(=O)C1COC(C)(C)O1

Mol. weight [g/mol]: 160.17

CAS: 52373-72-5

Physical Properties

Property code	Value	Unit	Source
gf	-374.75	kJ/mol	Joback Method
hf	-641.23	kJ/mol	Joback Method
hfus	21.34	kJ/mol	Joback Method
hvap	48.15	kJ/mol	Joback Method
log10ws	-0.40		Crippen Method
logp	0.311		Crippen Method
mcvol	117.810	ml/mol	McGowan Method
pc	3585.64	kPa	Joback Method
rinpol	1034.50		NIST Webbook
tb	500.60	K	Joback Method
tc	713.50	K	Joback Method
tf	324.51	K	Joback Method
vc	0.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.60	J/mol×K	500.60	Joback Method
cpg	293.98	J/mol×K	536.08	Joback Method
cpg	306.56	J/mol×K	571.57	Joback Method
cpg	318.40	J/mol×K	607.05	Joback Method

cpg	329.60	J/mol×K	642.53	Joback Method
cpg	340.23	J/mol×K	678.01	Joback Method
cpg	350.37	J/mol×K	713.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52373725&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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume