

1-(2,2-Dimethyl-1,3-dioxolan-4-yl)-2-methoxy-2-oxo- (E)-2-methylbut-2-enoate

InChIKey:

AVJFEIXNLVTSEZ-SOFGYWHQSA-N

Formula:

C₁₃H₂₀O₆

SMILES:

CC=C(C)C(=O)OC(C(=O)OC)C1COC(C)(C)O1

Mol. weight [g/mol]:

272.29

Physical Properties

Property code	Value	Unit	Source
gf	-488.92	kJ/mol	Joback Method
hf	-907.72	kJ/mol	Joback Method
hfus	35.03	kJ/mol	Joback Method
hvap	70.31	kJ/mol	Joback Method
log10ws	-1.74		Crippen Method
logp	1.189		Crippen Method
mcvol	205.490	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
rinpol	1659.00		NIST Webbook
rinpol	1659.00		NIST Webbook
tb	717.77	K	Joback Method
tc	931.67	K	Joback Method
tf	430.25	K	Joback Method
vc	0.766	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.09	J/mol×K	717.77	Joback Method
cpg	615.07	J/mol×K	753.42	Joback Method
cpg	630.33	J/mol×K	789.07	Joback Method
cpg	644.97	J/mol×K	824.72	Joback Method
cpg	659.07	J/mol×K	860.37	Joback Method
cpg	672.75	J/mol×K	896.02	Joback Method
cpg	686.08	J/mol×K	931.67	Joback Method

Sources

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=U373764&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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