1,3-Dioxolane-2-acetic acid, 2,4-dimethyl-, ethyl ester

Other names: Acetoacetic acid, ethyl ester, 1,2-propylene ketal
Ethyl 2,4-dimethyl-1,3-dioxolane-2-acetate
Ethylacetoacetate propyleneglycol ketal

Inchi: InChI=1S/C9H16O4/c1-3-11-8(10)7-9(2)12-5-4-6-13-9/h3-7H2,1-2H3

InchiKey: XMLLBDKQPQZGDP-UHFFFAOYSA-N

Formula: C9H16O4

SMILES: CCOC(=O)CC1(C)OCCCO1

Mol. weight [g/mol]: 188.22

CAS: 6290-17-1

Physical Properties

Property code	Value	Unit	Source
gf	-362.30	kJ/mol	Joback Method
hf	-668.33	kJ/mol	Joback Method
hfus	23.35	kJ/mol	Joback Method
hvap	53.08	kJ/mol	Joback Method
log10ws	-1.13		Crippen Method
logp	1.093		Crippen Method
mcvol	145.990	ml/mol	McGowan Method
pc	3072.75	kPa	Joback Method
tb	555.30	K	Joback Method
tc	769.11	K	Joback Method
tf	347.77	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.35	J/mol×K	555.30	Joback Method
cpg	385.91	J/mol×K	590.93	Joback Method
cpg	400.58	J/mol×K	626.57	Joback Method
cpg	414.44	J/mol×K	662.20	Joback Method
cpg	427.59	J/mol×K	697.84	Joback Method
cpg	440.11	J/mol×K	733.47	Joback Method

cpg	452.09	J/mol×K	769.11	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6290171&Units=SI

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