.alpha.-Acetyl-.alpha.-methyl-gammabutyrolacton

Other names: «alpha»-Acetyl-«alpha»-methyl-gammabutyrolactone
«alpha»-acetyl-«alpha»-methyl-«gamma»-butyrolactone
Inchi: InChI=1S/C7H10O3/c1-5(8)7(2)3-4-10-6(7)9/h3-4H2,1-2H3
InchiKey: VKDGCPFTXXDWQJ-UHFFFAOYSA-N
Formula: C7H10O3
SMILES: CC(=O)C1(C)CCOC1=O
Mol. weight [g/mol]: 142.15

Physical Properties

Property code	Value	Unit	Source
hfus	10.61	kJ/mol	Joback Method
logp	0.529		Crippen Method
mcvol	107.640	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.89	J/mol×K	523.72	Joback Method
cpg	264.96	J/mol×K	562.65	Joback Method
cpg	277.22	J/mol×K	601.58	Joback Method
cpg	288.75	J/mol×K	640.51	Joback Method
cpg	299.66	J/mol×K	679.44	Joback Method
cpg	310.06	J/mol×K	718.37	Joback Method
cpg	320.03	J/mol×K	757.30	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	370.50 ± 2.50	K	0.70	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1123199&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure