C7H10O4

Inchi: InChI=1S/C7H10O4/c1-10-6(8)4-3-5(4)7(9)11-2/h4-5H,3H2,1-2H3
InchiKey: JBVOSZYUSFDYIN-UHFFFAOYSA-N
Formula: C7H10O4
SMILES: COC(=O)C1CC1C(=O)OC
Mol. weight [g/mol]: 158.15
CAS: 826-34-6

Physical Properties

Property code	Value	Unit	Source
gf	-406.74	kJ/mol	Joback Method
hf	-624.95	kJ/mol	Joback Method
hfus	18.67	kJ/mol	Joback Method
hvap	49.09	kJ/mol	Joback Method
log10ws	0.11		Crippen Method
logp	-0.032		Crippen Method
mcvol	113.510	ml/mol	McGowan Method
pc	3456.14	kPa	Joback Method
tb	514.21	K	Joback Method
tc	713.66	K	Joback Method
tf	326.67	K	Joback Method
vc	0.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.77	J/mol×K	514.21	Joback Method
cpg	276.25	J/mol×K	547.45	Joback Method
cpg	287.21	J/mol×K	580.69	Joback Method
cpg	297.65	J/mol×K	613.94	Joback Method
cpg	307.57	J/mol×K	647.18	Joback Method
cpg	316.97	J/mol×K	680.42	Joback Method
cpg	325.87	J/mol×K	713.66	Joback Method
dvisc	0.0015664	Pa×s	326.67	Joback Method
dvisc	0.0012175	Pa×s	357.93	Joback Method

dvisc	0.0009854	Pa×s	389.18	Joback Method
dvisc	0.0008230	Pa×s	420.44	Joback Method
dvisc	0.0007048	Pa×s	451.70	Joback Method
dvisc	0.0006157	Pa×s	482.95	Joback Method
dvisc	0.0005468	Pa×s	514.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C826346&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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