Methyl 2,3-dimethoxy-3-butenoate

Inchi: InChI=1S/C7H12O4/c1-5(9-2)6(10-3)7(8)11-4/h6H,1H2,2-4H3
InchiKey: JHQCIXLLYZYJQW-UHFFFAOYSA-N
Formula: C7H12O4
SMILES: C=C(OC)C(OC)C(=O)OC
Mol. weight [g/mol]: 160.17
CAS: 82481-25-2

Physical Properties

Property code	Value	Unit	Source
gf	-359.01	kJ/mol	Joback Method
hf	-586.69	kJ/mol	Joback Method
hfus	12.94	kJ/mol	Joback Method
hvap	44.17	kJ/mol	Joback Method
log10ws	-0.25		Crippen Method
logp	0.335		Crippen Method
mcvol	124.370	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
tb	476.81	K	Joback Method
tc	662.96	K	Joback Method
tf	254.55	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.79	J/mol×K	476.81	Joback Method
cpg	278.46	J/mol×K	507.84	Joback Method
cpg	288.82	J/mol×K	538.86	Joback Method
cpg	298.85	J/mol×K	569.89	Joback Method
cpg	308.55	J/mol×K	600.91	Joback Method
cpg	317.90	J/mol×K	631.94	Joback Method
cpg	326.88	J/mol×K	662.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C82481252&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume