2-Butenoic acid, 2,3-dimethoxy-, methyl ester, (E)-

Inchi: InChI=1S/C7H12O4/c1-5(9-2)6(10-3)7(8)11-4/h1-4H3/b6-5+
InchiKey: WBGVTICYNBRHRL-AATRIKPKSA-N
Formula: C7H12O4
SMILES: COC(=O)C(OC)=C(C)OC
Mol. weight [g/mol]: 160.17
CAS: 82481-27-4

Physical Properties

Property code	Value	Unit	Source
gf	-372.74	kJ/mol	Joback Method
hf	-599.41	kJ/mol	Joback Method
hfus	16.63	kJ/mol	Joback Method
hvap	45.27	kJ/mol	Joback Method
log10ws	-0.63		Crippen Method
logp	0.684		Crippen Method
mcvol	124.370	ml/mol	McGowan Method
pc	3032.27	kPa	Joback Method
tb	484.61	K	Joback Method
tc	674.92	K	Joback Method
tf	252.27	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.38	J/mol×K	484.61	Joback Method
cpg	278.14	J/mol×K	516.33	Joback Method
cpg	288.56	J/mol×K	548.05	Joback Method
cpg	298.63	J/mol×K	579.77	Joback Method
cpg	308.33	J/mol×K	611.49	Joback Method
cpg	317.66	J/mol×K	643.20	Joback Method
cpg	326.60	J/mol×K	674.92	Joback Method

Sources

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=C82481274&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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