Dimethyl 2,3-dimethoxybutenedioate

Inchi: InChI=1S/C8H12O6/c1-11-5(7(9)13-3)6(12-2)8(10)14-4/h1-4H3/b6-5+
InchiKey: INFWEJMOAFPDCK-AATRIKPKSA-N
Formula: C8H12O6
SMILES: COC(=O)C(OC)=C(OC)C(=O)OC
Mol. weight [g/mol]: 204.18

Physical Properties

Property code	Value	Unit	Source
gf	-598.24	kJ/mol	Joback Method
hf	-864.85	kJ/mol	Joback Method
hfus	22.01	kJ/mol	Joback Method
hvap	56.65	kJ/mol	Joback Method
log10ws	0.09		Crippen Method
logp	-0.163		Crippen Method
mcvol	145.900	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
rinpol	1413.00		NIST Webbook
tb	583.78	K	Joback Method
tc	778.93	K	Joback Method
tf	335.70	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.38	J/mol×K	583.78	Joback Method
cpg	360.51	J/mol×K	616.30	Joback Method
cpg	371.20	J/mol×K	648.83	Joback Method
cpg	381.44	J/mol×K	681.35	Joback Method
cpg	391.19	J/mol×K	713.88	Joback Method
cpg	400.44	J/mol×K	746.40	Joback Method
cpg	409.17	J/mol×K	778.93	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=R80237&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume