2-Pentenedioic acid, 2-methoxy-, dimethyl ester

Other names: Dimethyl 2-methoxy-2-pentenedioate
2-Methoxy-pent-2-enedioic acid dimethyl ester
2-Pentenedioic acid, 2-methoxy-, 1,5-dimethyl ester
Inchi: InChI=1S/C8H12O5/c1-11-6(8(10)13-3)4-5-7(9)12-2/h4H,5H2,1-3H3/b6-4-
InchiKey: VKPFVKSMNVODAO-XQRVVYSFSA-N
Formula: C8H12O5
SMILES: COC(=O)CC=C(OC)C(=O)OC
Mol. weight [g/mol]: 188.18
CAS: 56009-33-7

Physical Properties

Property code	Value	Unit	Source
gf	-484.69	kJ/mol	Joback Method
hf	-722.84	kJ/mol	Joback Method
hfus	22.13	kJ/mol	Joback Method
hvap	54.16	kJ/mol	Joback Method
log10ws	-0.33		Crippen Method
logp	0.253		Crippen Method
mcvol	140.030	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
rinpol	1291.00		NIST Webbook
rinpol	1291.00		NIST Webbook
tb	561.48	K	Joback Method
tc	754.94	K	Joback Method
tf	327.43	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.33	J/mol×K	561.48	Joback Method
cpg	337.36	J/mol×K	593.72	Joback Method
cpg	347.94	J/mol×K	625.97	Joback Method
cpg	358.07	J/mol×K	658.21	Joback Method

cpg	367.72	J/mol×K	690.45	Joback Method
cpg	376.90	J/mol×K	722.69	Joback Method
cpg	385.60	J/mol×K	754.94	Joback Method

Sources

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=C56009337&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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