2-Methoxycarbonyl-pent-2-enedioic acid dimethyl ester

Inchi: InChI=1S/C9H12O6/c1-13-7(10)5-4-6(8(11)14-2)9(12)15-3/h4H,5H2,1-3H3
InchiKey: GNFDSUXUHQEDHK-UHFFFAOYSA-N
Formula: C9H12O6
SMILES: COC(=O)CC=C(C(=O)OC)C(=O)OC
Mol. weight [g/mol]: 216.19

Physical Properties

Property code	Value	Unit	Source
gf	-605.19	kJ/mol	Joback Method
hf	-856.06	kJ/mol	Joback Method
hfus	26.32	kJ/mol	Joback Method
hvap	63.13	kJ/mol	Joback Method
log10ws	-0.03		Crippen Method
logp	-0.178		Crippen Method
mcvol	155.690	ml/mol	McGowan Method
pc	2808.38	kPa	Joback Method
rinpol	1395.00		NIST Webbook
tb	638.23	K	Joback Method
tc	836.65	K	Joback Method
tf	388.63	K	Joback Method
vc	0.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.26	J/mol×K	638.23	Joback Method
cpg	398.25	J/mol×K	671.30	Joback Method
cpg	408.67	J/mol×K	704.37	Joback Method
cpg	418.53	J/mol×K	737.44	Joback Method
cpg	427.81	J/mol×K	770.51	Joback Method
cpg	436.49	J/mol×K	803.58	Joback Method
cpg	444.57	J/mol×K	836.65	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=R247740&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume