Hexanedioic acid, 2,4-dimethyl, dimethyl ester

Inchi: InChI=1S/C10H14O4/c1-7(6-9(11)13-3)5-8(2)10(12)14-4/h5-6H,1-4H3/b7-6+,8-5+
InchiKey: QIRTYCZMBXBUDU-ZCOYIIAOSA-N
Formula: C10H14O4
SMILES: COC(=O)C=C(C)C=C(C)C(=O)OC
Mol. weight [g/mol]: 198.22

Physical Properties

Property code	Value	Unit	Source
gf	-291.18	kJ/mol	Joback Method
hf	-524.47	kJ/mol	Joback Method
hfus	25.01	kJ/mol	Joback Method
hvap	56.24	kJ/mol	Joback Method
log10ws	-1.44		Crippen Method
logp	1.225		Crippen Method
mcvol	158.040	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
rinpol	1272.00		NIST Webbook
rinpol	1272.00		NIST Webbook
tb	588.86	K	Joback Method
tc	790.04	K	Joback Method
tf	308.70	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.39	J/mol×K	588.86	Joback Method
cpg	387.90	J/mol×K	622.39	Joback Method
cpg	399.77	J/mol×K	655.92	Joback Method
cpg	411.02	J/mol×K	689.45	Joback Method
cpg	421.65	J/mol×K	722.98	Joback Method
cpg	431.70	J/mol×K	756.51	Joback Method
cpg	441.17	J/mol×K	790.04	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=R106624&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