Hexanedioic acid, 2-methyl-5-methylene-, dimethyl ester

Other names: Dimethyl ester of 2-methyl-5-methylene-1,6-hexanedioic acid
dimethyl 2-methyl-5-methyleneadipate

Inchi: InChI=1S/C10H16O4/c1-7(9(11)13-3)5-6-8(2)10(12)14-4/h8H,1,5-6H2,2-4H3

InchiKey: SUISJNPVANLQPB-UHFFFAOYSA-N

Formula: C10H16O4

SMILES: C=C(CCC(C)C(=O)OC)C(=O)OC

Mol. weight [g/mol]: 200.23

CAS: 4513-62-6

Physical Properties

Property code	Value	Unit	Source
gf	-357.67	kJ/mol	Joback Method
hf	-628.97	kJ/mol	Joback Method
hfus	21.12	kJ/mol	Joback Method
hvap	55.19	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	1.305		Crippen Method
mcvol	162.340	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
tb	576.90	K	Joback Method
tc	766.55	K	Joback Method
tf	316.06	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.54	J/mol×K	576.90	Joback Method
cpg	408.60	J/mol×K	608.51	Joback Method
cpg	421.08	J/mol×K	640.12	Joback Method
cpg	432.97	J/mol×K	671.72	Joback Method
cpg	444.29	J/mol×K	703.33	Joback Method
cpg	455.02	J/mol×K	734.94	Joback Method
cpg	465.16	J/mol×K	766.55	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=C4513626&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume