HEPTANEDIOIC ACID, 2,4-DIMETHYL-, DIMETHYL ESTER

Inchi: InChI=1S/C11H20O4/c1-8(5-6-10(12)14-3)7-9(2)11(13)15-4/h8-9H,5-7H2,1-4H3
InchiKey: TZCQHHKPFVFJGT-UHFFFAOYSA-N
Formula: C11H20O4
SMILES: COC(=O)CCC(C)CC(C)C(=O)OC
Mol. weight [g/mol]: 216.28

Physical Properties

Property code	Value	Unit	Source
af	0.6235		Cheméo Relay (1.0)
hf	-887.22	kJ/mol	Cheméo Relay (1.0)
hfus	22.77	kJ/mol	Joback Method
hvap	73.24	kJ/mol	Cheméo Relay (1.0)
ie	9.49	eV	Cheméo Relay (1.0)
log10ws	-2.17		Cheméo Relay (1.0)
logp	1.775		Crippen Method
mcvol	180.730	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
tb	502.76	K	Cheméo Relay (1.0)
tc	682.52	K	Cheméo Relay (1.0)
tf	237.57	K	Cheméo Relay (1.0)
vc	0.653	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.83	J/mol×K	602.78	Joback Method
cpg	480.33	J/mol×K	633.59	Joback Method
cpg	494.18	J/mol×K	664.41	Joback Method
cpg	507.38	J/mol×K	695.22	Joback Method
cpg	519.94	J/mol×K	726.03	Joback Method
cpg	531.86	J/mol×K	756.85	Joback Method
cpg	543.12	J/mol×K	787.66	Joback Method
dvisc	0.0029767	Pa×s	328.05	Joback Method
dvisc	0.0013297	Pa×s	373.84	Joback Method

dvisc	0.0007082	Pa×s	419.63	Joback Method
dvisc	0.0004269	Pa×s	465.41	Joback Method
dvisc	0.0002818	Pa×s	511.20	Joback Method
dvisc	0.0001992	Pa×s	556.99	Joback Method
dvisc	0.0001484	Pa×s	602.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72719041&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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