Hexanoic acid, 3,5,5-trimethyl-, methyl ester

Inchi: InChI=1S/C10H20O2/c1-8(6-9(11)12-5)7-10(2,3)4/h8H,6-7H2,1-5H3
InchiKey: DCPCIGBOUDWJEZ-UHFFFAOYSA-N
Formula: C10H20O2
SMILES: COC(=O)CC(C)CC(C)(C)C
Mol. weight [g/mol]: 172.26

Physical Properties

Property code	Value	Unit	Source
gf	-200.20	kJ/mol	Joback Method
hf	-508.56	kJ/mol	Joback Method
hfus	13.51	kJ/mol	Joback Method
hvap	45.33	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.622		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
rinpol	1082.00		NIST Webbook
tb	500.82	K	Joback Method
tc	686.98	K	Joback Method
tf	262.04	K	Joback Method
vc	0.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.17	J/mol×K	500.82	Joback Method
cpg	386.77	J/mol×K	531.85	Joback Method
cpg	401.63	J/mol×K	562.87	Joback Method
cpg	415.78	J/mol×K	593.90	Joback Method
cpg	429.24	J/mol×K	624.93	Joback Method
cpg	442.02	J/mol×K	655.96	Joback Method
cpg	454.15	J/mol×K	686.98	Joback Method
dvisc	0.0064596	Pa×s	262.04	Joback Method
dvisc	0.0024849	Pa×s	301.84	Joback Method

dvisc	0.0011942	Pa×s	341.63	Joback Method
dvisc	0.0006687	Pa×s	381.43	Joback Method
dvisc	0.0004178	Pa×s	421.23	Joback Method
dvisc	0.0002831	Pa×s	461.02	Joback Method
dvisc	0.0002041	Pa×s	500.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406049&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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