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

Inchi: InChI=1S/C11H22O2/c1-6-13-10(12)7-9(2)8-11(3,4)5/h9H,6-8H2,1-5H3
InchiKey: NMZMQQBBZRGLPJ-UHFFFAOYSA-N
Formula: C11H22O2
SMILES: CCOC(=O)CC(C)CC(C)(C)C
Mol. weight [g/mol]: 186.29

Physical Properties

Property code	Value	Unit	Source
gf	-191.78	kJ/mol	Joback Method
hf	-529.20	kJ/mol	Joback Method
hfus	16.10	kJ/mol	Joback Method
hvap	47.55	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	3.012		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
rinpol	1151.00		NIST Webbook
rinpol	1151.00		NIST Webbook
tb	523.70	K	Joback Method
tc	707.84	K	Joback Method
tf	273.31	K	Joback Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.38	J/mol×K	523.70	Joback Method
cpg	434.70	J/mol×K	554.39	Joback Method
cpg	450.26	J/mol×K	585.08	Joback Method
cpg	465.08	J/mol×K	615.77	Joback Method
cpg	479.16	J/mol×K	646.46	Joback Method
cpg	492.55	J/mol×K	677.15	Joback Method
cpg	505.25	J/mol×K	707.84	Joback Method
dvisc	0.0059930	Pa×s	273.31	Joback Method

dvisc	0.0022813	Pa×s	315.04	Joback Method
dvisc	0.0010885	Pa×s	356.77	Joback Method
dvisc	0.0006065	Pa×s	398.50	Joback Method
dvisc	0.0003775	Pa×s	440.24	Joback Method
dvisc	0.0002551	Pa×s	481.97	Joback Method
dvisc	0.0001835	Pa×s	523.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406050&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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