Hexanoic acid, 3,5,5-trimethyl-, 4-methyl-2-pentyl ester

Inchi: InChI=1S/C15H30O2/c1-11(2)8-13(4)17-14(16)9-12(3)10-15(5,6)7/h11-13H,8-10H2,1-7H

InchiKey: LLGLURCCPYKGIJ-UHFFFAOYSA-N

Formula: C15H30O2

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

Mol. weight [g/mol]: 242.40

Physical Properties

Property code	Value	Unit	Source
gf	-162.98	kJ/mol	Joback Method
hf	-622.32	kJ/mol	Joback Method
hfus	19.41	kJ/mol	Joback Method
hvap	55.68	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.427		Crippen Method
mcvol	229.650	ml/mol	McGowan Method
pc	1515.21	kPa	Joback Method
rinpol	1439.00		NIST Webbook
rinpol	1439.00		NIST Webbook
tb	614.34	K	Joback Method
tc	797.87	K	Joback Method
tf	288.39	K	Joback Method
vc	0.871	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.39	J/mol×K	614.34	Joback Method
cpg	643.52	J/mol×K	644.93	Joback Method
cpg	661.70	J/mol×K	675.52	Joback Method
cpg	678.96	J/mol×K	706.10	Joback Method
cpg	695.32	J/mol×K	736.69	Joback Method
cpg	710.83	J/mol×K	767.28	Joback Method
cpg	725.51	J/mol×K	797.87	Joback Method
dvisc	0.0088187	Pa×s	288.39	Joback Method

dvisc	0.0023000	Pa×s	342.71	Joback Method
dvisc	0.0008665	Pa×s	397.04	Joback Method
dvisc	0.0004129	Pa×s	451.37	Joback Method
dvisc	0.0002307	Pa×s	505.69	Joback Method
dvisc	0.0001444	Pa×s	560.02	Joback Method
dvisc	0.0000981	Pa×s	614.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406056&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