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

Inchi: InChI=1S/C12H24O2/c1-9(2)14-11(13)7-10(3)8-12(4,5)6/h9-10H,7-8H2,1-6H3
InchiKey: DPRDCWLARMPWSR-UHFFFAOYSA-N
Formula: C12H24O2
SMILES: CC(CC(=O)OC(C)C)CC(C)(C)C
Mol. weight [g/mol]: 200.32

Physical Properties

Property code	Value	Unit	Source
gf	-185.80	kJ/mol	Joback Method
hf	-555.12	kJ/mol	Joback Method
hfus	15.16	kJ/mol	Joback Method
hvap	49.39	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.400		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1908.57	kPa	Joback Method
rinpol	1184.00		NIST Webbook
tb	546.14	K	Joback Method
tc	731.94	K	Joback Method
tf	269.58	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.59	J/mol×K	546.14	Joback Method
cpg	484.95	J/mol×K	577.11	Joback Method
cpg	501.47	J/mol×K	608.07	Joback Method
cpg	517.18	J/mol×K	639.04	Joback Method
cpg	532.09	J/mol×K	670.00	Joback Method
cpg	546.24	J/mol×K	700.97	Joback Method
cpg	559.65	J/mol×K	731.94	Joback Method
dvisc	0.0083365	Pa×s	269.58	Joback Method
dvisc	0.0026373	Pa×s	315.67	Joback Method

dvisc	0.0011187	Pa×s	361.77	Joback Method
dvisc	0.0005760	Pa×s	407.86	Joback Method
dvisc	0.0003394	Pa×s	453.95	Joback Method
dvisc	0.0002205	Pa×s	500.05	Joback Method
dvisc	0.0001540	Pa×s	546.14	Joback Method

Sources

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=U406051&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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