Hexanoic acid, 1,1-dimethylethyl ester

Other names: tert-butyl hexanoate
Inchi: InChI=1S/C10H20O2/c1-5-6-7-8-9(11)12-10(2,3)4/h5-8H2,1-4H3
InchiKey: DANUJARGWMPVQX-UHFFFAOYSA-N
Formula: C10H20O2
SMILES: CCCCCC(=O)OC(C)(C)C
Mol. weight [g/mol]: 172.26
CAS: 2492-18-4

Physical Properties

Property code	Value	Unit	Source
gf	-197.76	kJ/mol	Joback Method
hf	-503.28	kJ/mol	Joback Method
hfus	17.03	kJ/mol	Joback Method
hvap	45.71	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.908		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	1060.00		NIST Webbook
rinpol	1055.00		NIST Webbook
ripol	1227.00		NIST Webbook
tb	501.26	K	Joback Method
tc	683.58	K	Joback Method
tf	277.04	K	Joback Method
vc	0.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.98	J/mol×K	501.26	Joback Method
cpg	440.23	J/mol×K	653.19	Joback Method
cpg	427.70	J/mol×K	622.81	Joback Method
cpg	414.52	J/mol×K	592.42	Joback Method
cpg	400.69	J/mol×K	562.03	Joback Method

cpg	386.18	J/mol×K	531.65	Joback Method
cpg	452.15	J/mol×K	683.58	Joback Method
dvisc	0.0002157	Pa×s	501.26	Joback Method
dvisc	0.0002909	Pa×s	463.89	Joback Method
dvisc	0.0004134	Pa×s	426.52	Joback Method
dvisc	0.0006286	Pa×s	389.15	Joback Method
dvisc	0.0010446	Pa×s	351.78	Joback Method
dvisc	0.0019589	Pa×s	314.41	Joback Method
dvisc	0.0043525	Pa×s	277.04	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2492184&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume