hexanoic acid, 1-methylpropyl ester

Inchi: InChI=1S/C10H20O2/c1-4-6-7-8-10(11)12-9(3)5-2/h9H,4-8H2,1-3H3
InchiKey: XVTUSVZMEFPBMT-UHFFFAOYSA-N
Formula: C10H20O2
SMILES: CCCCCC(=O)OC(C)CC
Mol. weight [g/mol]: 172.26
CAS: 820-00-8

Physical Properties

Property code	Value	Unit	Source
af	0.5788		Cheméo Relay (1.0)
hf	-598.39	kJ/mol	Cheméo Relay (1.0)
hfus	20.92	kJ/mol	Joback Method
hvap	52.94	kJ/mol	Cheméo Relay (1.0)
ie	9.70	eV	Cheméo Relay (1.0)
log10ws	-2.82		Cheméo Relay (1.0)
logp	2.908		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
tb	445.37	K	Cheméo Relay (1.0)
tc	634.74	K	Cheméo Relay (1.0)
tf	205.29	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.31	J/mol×K	504.05	Joback Method
cpg	382.82	J/mol×K	533.34	Joback Method
cpg	396.77	J/mol×K	562.64	Joback Method
cpg	410.17	J/mol×K	591.93	Joback Method
cpg	423.03	J/mol×K	621.22	Joback Method
cpg	435.35	J/mol×K	650.52	Joback Method
cpg	447.14	J/mol×K	679.81	Joback Method
dvisc	0.0046674	Pa×s	259.62	Joback Method
dvisc	0.0019627	Pa×s	300.36	Joback Method

dvisc	0.0010151	Pa×s	341.10	Joback Method
dvisc	0.0006043	Pa×s	381.83	Joback Method
dvisc	0.0003976	Pa×s	422.57	Joback Method
dvisc	0.0002816	Pa×s	463.31	Joback Method
dvisc	0.0002109	Pa×s	504.05	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C820008&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point