Hexanoic acid, 1-methylethyl ester

Other names:	Hexanoic acid, isopropyl ester
	Isopropyl hexanoate
	n-C5H11C(O)OCH(CH3)2
	n-Caproic acid isopropyl ester
	iso-Propyl n-hexanoate
	Isopropyl caproate
Inchi:	InChI=1S/C9H18O2/c1-4-5-6-7-9(10)11-8(2)3/h8H,4-7H2,1-3H3
InchiKey:	JSHDAORXSNJOBA-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CCCCCC(=O)OC(C)C
Mol. weight [g/mol]:	158.24
CAS:	2311-46-8

Physical Properties

Property code	Value	Unit	Source
gf	-211.46	kJ/mol	Joback Method
hf	-479.17	kJ/mol	Joback Method
hfus	18.33	kJ/mol	Joback Method
hvap	44.40	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.518		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
rinpol	1008.00		NIST Webbook
rinpol	1046.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	1026.00		NIST Webbook

rinpol	1008.00		NIST Webbook
rinpol	1022.00		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1022.00		NIST Webbook
ripol	1236.00		NIST Webbook
ripol	1228.00		NIST Webbook
ripol	1223.00		NIST Webbook
ripol	1236.00		NIST Webbook
ripol	1228.00		NIST Webbook
tb	481.17	K	Joback Method
tc	658.49	K	Joback Method
tf	248.35	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.06	J/mol×K	481.17	Joback Method
cpg	336.66	J/mol×K	510.72	Joback Method
cpg	349.76	J/mol×K	540.28	Joback Method
cpg	362.35	J/mol×K	569.83	Joback Method
cpg	374.44	J/mol×K	599.38	Joback Method
cpg	386.04	J/mol×K	628.93	Joback Method
cpg	397.15	J/mol×K	658.49	Joback Method
dvisc	0.0047844	Pa×s	248.35	Joback Method
dvisc	0.0020429	Pa×s	287.15	Joback Method
dvisc	0.0010682	Pa×s	325.96	Joback Method
dvisc	0.0006412	Pa×s	364.76	Joback Method
dvisc	0.0004246	Pa×s	403.56	Joback Method
dvisc	0.0003022	Pa×s	442.37	Joback Method
dvisc	0.0002272	Pa×s	481.17	Joback Method
hvapt	51.60	kJ/mol	345.00	NIST Webbook

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=C2311468&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
hvapt:	Enthalpy of vaporization at a given temperature
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