

Hexanoic acid, 1-methylbutyl ester

Other names:	2-pentyl hexanoate isopentyl hexanoate
Inchi:	InChI=1S/C11H22O2/c1-4-6-7-9-11(12)13-10(3)8-5-2/h10H,4-9H2,1-3H3
InchiKey:	LDSKHRQOZJYTFX-UHFFFAOYSA-N
Formula:	C11H22O2
SMILES:	CCCCC(=O)OC(C)CCC
Mol. weight [g/mol]:	186.29
CAS:	88164-61-8

Physical Properties

Property code	Value	Unit	Source
gf	-194.62	kJ/mol	Joback Method
hf	-520.45	kJ/mol	Joback Method
hfus	23.51	kJ/mol	Joback Method
hvap	48.85	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	3.298		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
ripol	1397.00		NIST Webbook
ripol	1407.00		NIST Webbook
ripol	1407.00		NIST Webbook
tb	526.93	K	Joback Method
tc	701.19	K	Joback Method
tf	270.89	K	Joback Method
vc	0.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.48	J/mol×K	526.93	Joback Method
cpg	430.78	J/mol×K	555.97	Joback Method
cpg	445.49	J/mol×K	585.02	Joback Method
cpg	459.60	J/mol×K	614.06	Joback Method

cpg	473.13	J/mol×K	643.11	Joback Method
cpg	486.09	J/mol×K	672.15	Joback Method
cpg	498.48	J/mol×K	701.19	Joback Method
dvisc	0.0044896	Pa×s	270.89	Joback Method
dvisc	0.0018616	Pa×s	313.56	Joback Method
dvisc	0.0009531	Pa×s	356.24	Joback Method
dvisc	0.0005632	Pa×s	398.91	Joback Method
dvisc	0.0003684	Pa×s	441.58	Joback Method
dvisc	0.0002597	Pa×s	484.26	Joback Method
dvisc	0.0001937	Pa×s	526.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88164618&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

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

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