Nonanoic acid, 3-methylbutyl ester

Other names:	Isoamyl nonoate
	Nonanoic acid, isopentyl ester
	isoamyl nonanoate
	isopentyl nonanoate
Inchi:	InChI=1S/C14H28O2/c1-4-5-6-7-8-9-10-14(15)16-12-11-13(2)3/h13H,4-12H2,1-3H3
InchiKey:	SHGMLOSSRPFLKG-UHFFFAOYSA-N
Formula:	C14H28O2
SMILES:	CCCCCCCCC(=O)OCCC(C)C
Mol. weight [g/mol]:	228.37
CAS:	7779-70-6

Physical Properties

Property code	Value	Unit	Source
gf	-169.36	kJ/mol	Joback Method
hf	-582.37	kJ/mol	Joback Method
hfus	31.28	kJ/mol	Joback Method
hvap	55.53	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	4.326		Crippen Method
mcvol	215.560	ml/mol	McGowan Method
pc	1589.81	kPa	Joback Method
rinpol	1559.00		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1527.00		NIST Webbook
ripol	1748.00		NIST Webbook
ripol	1748.00		NIST Webbook
ripol	1748.00		NIST Webbook
ripol	1752.00		NIST Webbook
tb	595.57	K	Joback Method
tc	766.26	K	Joback Method
tf	304.70	K	Joback Method
tt	233.20	K	Influence of Additives (Isoamyl Laurate or Isoamyl Nonanoate) in the Solid-Liquid Equilibrium of Fatty Acid Ethyl Esters
vc	0.838	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.35	J/mol×K	595.57	Joback Method
cpg	584.55	J/mol×K	624.02	Joback Method
cpg	601.04	J/mol×K	652.47	Joback Method
cpg	616.82	J/mol×K	680.91	Joback Method
cpg	631.92	J/mol×K	709.36	Joback Method
cpg	646.34	J/mol×K	737.81	Joback Method
cpg	660.10	J/mol×K	766.26	Joback Method
dvisc	0.0037349	Pa×s	304.70	Joback Method
dvisc	0.0014934	Pa×s	353.18	Joback Method
dvisc	0.0007451	Pa×s	401.66	Joback Method
dvisc	0.0004318	Pa×s	450.13	Joback Method
dvisc	0.0002782	Pa×s	498.61	Joback Method
dvisc	0.0001938	Pa×s	547.09	Joback Method
dvisc	0.0001432	Pa×s	595.57	Joback Method

Sources

Influence of Additives (Isoamyl Laurate or Isoamyl Nonanoate) in the Solid-Liquid Equilibrium of Fatty Acid Ethyl Esters:	https://www.doi.org/10.1021/acs.jced.8b01019
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=C7779706&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume