Isoamyl laurate

Other names:	3-Methylbutyl dodecanoate
	Dodecanoic acid, 3-methylbutyl ester
	Isoamyl dodecanoate
	Isopentyl laurate
	Lauric acid, isopentyl ester
	iso-Amyl n-dodecanoate
	isopentyl dodecanoate
Inchi:	InChI=1S/C17H34O2/c1-4-5-6-7-8-9-10-11-12-13-17(18)19-15-14-16(2)3/h16H,4-15H2,1
InchiKey:	FVKRIDSRWFEQME-UHFFFAOYSA-N
Formula:	C17H34O2
SMILES:	CCCCCCCCCCCC(=O)OCCC(C)C
Mol. weight [g/mol]:	270.45
CAS:	6309-51-9

Physical Properties

Property code	Value	Unit	Source
gf	-144.10	kJ/mol	Joback Method
hf	-644.29	kJ/mol	Joback Method
hfus	39.05	kJ/mol	Joback Method
hvap	62.20	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	5.497		Crippen Method
mcvol	257.830	ml/mol	McGowan Method
pc	1279.16	kPa	Joback Method
rinpol	1844.60		NIST Webbook
rinpol	1829.00		NIST Webbook
rinpol	1844.00		NIST Webbook
rinpol	1851.00		NIST Webbook
rinpol	1847.00		NIST Webbook
rinpol	1847.00		NIST Webbook
rinpol	1844.00		NIST Webbook
rinpol	1844.00		NIST Webbook
rinpol	1847.00		NIST Webbook
rinpol	1870.00		NIST Webbook
ripol	2110.00		NIST Webbook
ripol	2059.00		NIST Webbook
ripol	2066.00		NIST Webbook

ripol	2056.00		NIST Webbook
ripol	2048.00		NIST Webbook
ripol	2059.00		NIST Webbook
ripol	2071.00		NIST Webbook
ripol	2064.00		NIST Webbook
tb	664.21	K	Joback Method
tc	833.82	K	Joback Method
tf	338.51	K	Joback Method
tt	258.00	K	Influence of Additives (Isoamyl Laurate or Isoamyl Nonanoate) in the Solid-Liquid Equilibrium of Fatty Acid Ethyl Esters
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.67	J/mol×K	664.21	Joback Method
cpg	751.27	J/mol×K	692.48	Joback Method
cpg	769.05	J/mol×K	720.75	Joback Method
cpg	786.03	J/mol×K	749.02	Joback Method
cpg	802.22	J/mol×K	777.28	Joback Method
cpg	817.65	J/mol×K	805.55	Joback Method
cpg	832.34	J/mol×K	833.82	Joback Method
dvisc	0.0028787	Pa×s	338.51	Joback Method
dvisc	0.0011177	Pa×s	392.79	Joback Method
dvisc	0.0005461	Pa×s	447.08	Joback Method
dvisc	0.0003116	Pa×s	501.36	Joback Method
dvisc	0.0001983	Pa×s	555.64	Joback Method
dvisc	0.0001368	Pa×s	609.93	Joback Method
dvisc	0.0001003	Pa×s	664.21	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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=C6309519&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
tt:	Triple Point Temperature
vc:	Critical Volume