NONANOIC ACID, 1-METHYLETHYL ESTER

Other names: Isopropyl nonanoate
isopropyl nonan-1-oate
Inchi: InChI=1S/C12H24O2/c1-4-5-6-7-8-9-10-12(13)14-11(2)3/h11H,4-10H2,1-3H3
InchiKey: DVFZGWDMFKTMFQ-UHFFFAOYSA-N
Formula: C12H24O2
SMILES: CCCCCCCCC(=O)OC(C)C
Mol. weight [g/mol]: 200.32

Physical Properties

Property code	Value	Unit	Source
af	0.6545		Cheméo Relay (1.0)
hf	-630.20	kJ/mol	Cheméo Relay (1.0)
hfus	26.10	kJ/mol	Joback Method
hvap	61.39	kJ/mol	Cheméo Relay (1.0)
ie	9.65	eV	Cheméo Relay (1.0)
log10ws	-4.03		Cheméo Relay (1.0)
logp	3.689		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
rinpol	1318.00		NIST Webbook
ripol	1516.00		NIST Webbook
tb	470.23	K	Cheméo Relay (1.0)
tc	661.62	K	Cheméo Relay (1.0)
tf	239.22	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.44	J/mol×K	549.81	Joback Method
cpg	480.46	J/mol×K	578.62	Joback Method
cpg	495.83	J/mol×K	607.44	Joback Method
cpg	510.57	J/mol×K	636.25	Joback Method
cpg	524.69	J/mol×K	665.07	Joback Method
cpg	538.20	J/mol×K	693.88	Joback Method

cpg	551.11	J/mol×K	722.69	Joback Method
dvisc	0.0042661	Pa×s	282.16	Joback Method
dvisc	0.0017460	Pa×s	326.77	Joback Method
dvisc	0.0008857	Pa×s	371.38	Joback Method
dvisc	0.0005197	Pa×s	415.99	Joback Method
dvisc	0.0003381	Pa×s	460.59	Joback Method
dvisc	0.0002373	Pa×s	505.20	Joback Method
dvisc	0.0001764	Pa×s	549.81	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C28267325&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

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