Nonanoic acid, 3-methylbutyl-2 ester

Inchi: InChI=1S/C14H28O2/c1-5-6-7-8-9-10-11-14(15)16-13(4)12(2)3/h12-13H,5-11H2,1-4H3
InchiKey: HROZBGLNCSSSMV-UHFFFAOYSA-N
Formula: C14H28O2
SMILES: CCCCCCCCC(=O)OC(C)C(C)C
Mol. weight [g/mol]: 228.37

Physical Properties

Property code	Value	Unit	Source
gf	-171.80	kJ/mol	Joback Method
hf	-587.65	kJ/mol	Joback Method
hfus	27.76	kJ/mol	Joback Method
hvap	55.14	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	4.325		Crippen Method
mcvol	215.560	ml/mol	McGowan Method
pc	1600.00	kPa	Joback Method
rinpol	1506.00		NIST Webbook
rinpol	1506.00		NIST Webbook
tb	595.13	K	Joback Method
tc	768.62	K	Joback Method
tf	289.70	K	Joback Method
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.68	J/mol×K	595.13	Joback Method
cpg	648.02	J/mol×K	739.70	Joback Method
cpg	633.39	J/mol×K	710.79	Joback Method
cpg	618.05	J/mol×K	681.87	Joback Method
cpg	602.00	J/mol×K	652.96	Joback Method
cpg	585.21	J/mol×K	624.04	Joback Method
cpg	661.96	J/mol×K	768.62	Joback Method
dvisc	0.0001338	Pa×s	595.13	Joback Method

dvisc	0.0001853	Pa×s	544.23	Joback Method
dvisc	0.0002745	Pa×s	493.32	Joback Method
dvisc	0.0004451	Pa×s	442.42	Joback Method
dvisc	0.0008184	Pa×s	391.51	Joback Method
dvisc	0.0018054	Pa×s	340.61	Joback Method
dvisc	0.0052596	Pa×s	289.70	Joback Method

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=U360663&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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