Nonanoic acid, neopentyl ester

Other names: Nonoic acid, neopentyl ester
Inchi: InChI=1S/C14H28O2/c1-5-6-7-8-9-10-11-13(15)16-12-14(2,3)4/h5-12H2,1-4H3
InchiKey: HEUVBUBESLJSMH-UHFFFAOYSA-N
Formula: C14H28O2
SMILES: CCCCCCCCC(=O)OCC(C)(C)C
Mol. weight [g/mol]: 228.37

Physical Properties

Property code	Value	Unit	Source
gf	-164.08	kJ/mol	Joback Method
hf	-585.84	kJ/mol	Joback Method
hfus	27.39	kJ/mol	Joback Method
hvap	54.62	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	4.326		Crippen Method
mcvol	215.560	ml/mol	McGowan Method
pc	1603.85	kPa	Joback Method
rinpol	1481.00		NIST Webbook
rinpol	1481.00		NIST Webbook
tb	592.78	K	Joback Method
tc	768.58	K	Joback Method
tf	322.12	K	Joback Method
vc	0.833	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.76	J/mol×K	592.78	Joback Method
cpg	587.39	J/mol×K	622.08	Joback Method
cpg	604.22	J/mol×K	651.38	Joback Method
cpg	620.25	J/mol×K	680.68	Joback Method
cpg	635.52	J/mol×K	709.98	Joback Method
cpg	650.04	J/mol×K	739.28	Joback Method
cpg	663.85	J/mol×K	768.58	Joback Method

dvisc	0.0032737	Pa×s	322.12	Joback Method
dvisc	0.0013947	Pa×s	367.23	Joback Method
dvisc	0.0007161	Pa×s	412.34	Joback Method
dvisc	0.0004194	Pa×s	457.45	Joback Method
dvisc	0.0002703	Pa×s	502.56	Joback Method
dvisc	0.0001874	Pa×s	547.67	Joback Method
dvisc	0.0001373	Pa×s	592.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358021&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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