

Isovaleric acid, nonyl ester

Other names:	nonyl isovalerate
Inchi:	InChI=1S/C14H28O2/c1-4-5-6-7-8-9-10-11-16-14(15)12-13(2)3/h13H,4-12H2,1-3H3
InchiKey:	JHKZVDVMXZGMOX-UHFFFAOYSA-N
Formula:	C14H28O2
SMILES:	CCCCCCCCCOC(=O)CC(C)C
Mol. weight [g/mol]:	228.37
CAS:	7786-47-2

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	1558.00		NIST Webbook
rinpol	1558.00		NIST Webbook
tb	595.57	K	Joback Method
tc	766.26	K	Joback Method
tf	304.70	K	Joback Method
vc	0.838	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.35	J/molxK	595.57	Joback Method
cpg	584.55	J/molxK	624.02	Joback Method
cpg	601.04	J/molxK	652.47	Joback Method
cpg	616.82	J/molxK	680.91	Joback Method
cpg	631.92	J/molxK	709.36	Joback Method
cpg	646.34	J/molxK	737.81	Joback Method

cpg	660.10	J/molxK	766.26	Joback Method
dvisc	0.0037349	Paxs	304.70	Joback Method
dvisc	0.0014934	Paxs	353.18	Joback Method
dvisc	0.0007451	Paxs	401.66	Joback Method
dvisc	0.0004318	Paxs	450.13	Joback Method
dvisc	0.0002782	Paxs	498.61	Joback Method
dvisc	0.0001938	Paxs	547.09	Joback Method
dvisc	0.0001432	Paxs	595.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7786472&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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