Nonanoic acid, 2-methylpropyl ester

Other names:	Isobutyl nonoate
	Isobutyl nonanoate
	Nonanoic acid, isobutyl ester
	isobutyl nonan-1-oate
Inchi:	InChI=1S/C13H26O2/c1-4-5-6-7-8-9-10-13(14)15-11-12(2)3/h12H,4-11H2,1-3H3
InchiKey:	NVVLMTNIHQHZPR-UHFFFAOYSA-N
Formula:	C13H26O2
SMILES:	CCCCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]:	214.34
CAS:	30982-03-7

Physical Properties

Property code	Value	Unit	Source
gf	-177.78	kJ/mol	Joback Method
hf	-561.73	kJ/mol	Joback Method
hfus	28.69	kJ/mol	Joback Method
hvap	53.30	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.936		Crippen Method
mcvol	201.470	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
rinpol	1446.00		NIST Webbook
rinpol	1428.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1428.00		NIST Webbook
tb	572.69	K	Joback Method
tc	744.36	K	Joback Method
tf	293.43	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.10	J/mol×K	572.69	Joback Method

cpg	531.74	J/mol×K	601.30	Joback Method
cpg	547.70	J/mol×K	629.91	Joback Method
cpg	563.00	J/mol×K	658.53	Joback Method
cpg	577.64	J/mol×K	687.14	Joback Method
cpg	591.64	J/mol×K	715.75	Joback Method
cpg	605.00	J/mol×K	744.36	Joback Method
dvisc	0.0040106	Pa×s	293.43	Joback Method
dvisc	0.0016218	Pa×s	339.97	Joback Method
dvisc	0.0008156	Pa×s	386.52	Joback Method
dvisc	0.0004755	Pa×s	433.06	Joback Method
dvisc	0.0003078	Pa×s	479.60	Joback Method
dvisc	0.0002152	Pa×s	526.15	Joback Method
dvisc	0.0001594	Pa×s	572.69	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=C30982037&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