Nonanoic acid, 2-methylpentyl ester

Inchi: InChI=1S/C15H30O2/c1-4-6-7-8-9-10-12-15(16)17-13-14(3)11-5-2/h14H,4-13H2,1-3H3
InchiKey: FJKXBNRJUOBLDW-UHFFFAOYSA-N
Formula: C15H30O2
SMILES: CCCCCCCCC(=O)OCC(C)CCC
Mol. weight [g/mol]: 242.40

Physical Properties

Property code	Value	Unit	Source
gf	-160.94	kJ/mol	Joback Method
hf	-603.01	kJ/mol	Joback Method
hfus	33.87	kJ/mol	Joback Method
hvap	57.75	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.716		Crippen Method
mcvol	229.650	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
rinpol	1648.00		NIST Webbook
tb	618.45	K	Joback Method
tc	788.43	K	Joback Method
tf	315.97	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.09	J/mol×K	618.45	Joback Method
cpg	702.28	J/mol×K	760.10	Joback Method
cpg	687.48	J/mol×K	731.77	Joback Method
cpg	671.98	J/mol×K	703.44	Joback Method
cpg	655.75	J/mol×K	675.11	Joback Method
cpg	638.80	J/mol×K	646.78	Joback Method
cpg	716.38	J/mol×K	788.43	Joback Method
dvisc	0.0001278	Pa×s	618.45	Joback Method
dvisc	0.0001735	Pa×s	568.04	Joback Method

dvisc	0.0002499	Pa×s	517.62	Joback Method
dvisc	0.0003895	Pa×s	467.21	Joback Method
dvisc	0.0006759	Pa×s	416.80	Joback Method
dvisc	0.0013649	Pa×s	366.38	Joback Method
dvisc	0.0034492	Pa×s	315.97	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=U360666&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